

**APPLIED MATHEMATICS DIVISION
SUMMARY REPORT**

June 1972



U of C-AIA-USAEC

ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS

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SUMMARY REPORT

June 1972

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APPLIED MATHEMATICS DIVISION
SUMMARY REPORT

June 1972

ABSTRACT

This report covers the activities of the Applied Mathematics Division as of June 30, 1972. The report is intended to reflect our activities of primary importance to the programs of the U. S. Atomic Energy Commission and Argonne National Laboratory. The activities of FY 1971 and 1972 and highlights of the previous two years are described.

The principal activities reported are: computer research and development; our mathematics program, which has been focused on two main areas of investigation: mathematical physics and computational mathematics; programming research and collaborative research with other Argonne divisions.

Certain activities within our Computer Center are also described. Among them is the development of the RESCUE Timesharing System and the recent acquisition of an IBM/360 Model 195 computer system. In addition, the activities of the Argonne Code Center are reported.

1.0 INTRODUCTION

The Applied Mathematics Division has four objectives:

- 1) to conduct research in mathematics and computer science which will provide results, methods, and insights which will enhance Argonne and the Atomic Energy Commission's ability generally to perform calculations and particularly to use computers;
- 2) to conduct collaborative research with other ANL divisions which involve substantive amounts of mathematics and computer science;
- 3) to provide for the computational needs of the Laboratory by planning, developing and operating the necessary computational facilities and providing computer programming and mathematical support; and
- 4) to operate the Argonne Code Center for AEC-wide, national, and international distribution of computer programs.

This report describes the activities of FY1971 and 1972 and records the highlights of the previous two years. Recent changes in the programmatic direction of the Mathematics and Computer Branch of the AEC Division of Physical Research are affecting future directions of our research activities, particularly the elimination of the Computer Research and Development program. These changes have caused some activities to be eliminated and redirected

others in the direction of programming research (computer science). This report, however, describes past activities and so is organized around their structure rather than around our future plans.

The principal activities of the Computer Research and Development Program have been in image processing, computer systems performance measurement, and computer graphics and computer microstructure.

The Mathematics program has been focused on two main areas of investigation; mathematical physics, with particular emphasis on the neutron transport equation, and on computational mathematics, with a number of investigations within each area.

The Programming Research program has involved a lesser number of activities than our other programs. It has consisted of automated theorem proving, extensible languages, and language definition.

Collaborative Research includes a wide variety of work supported in a variety of ways. Some, like the Great Lakes Studies and the Argonne Braille Machine have involved AMD personnel in the original development of the proposal, while other work has been commissioned as an applied programming activity by another ANL division.

The Computer Center has operated the central computing facility and developed and implemented plans for the installation of new equipment. It has also developed various facilities, such as the RESCUE time sharing system, for use on the computer systems. The recent acquisition of an IBM/360 Model 195 computer further broadens our ability to achieve the objectives of the Laboratory.

The Argonne Code Center receives, assimilates and distributes codes and abstracts. It has developed a computer based system, ACCESS, to aid in performing this work. It has also undertaken cooperative standardization activities to further facilitate the exchange of codes.

2.0 DIVISIONAL ORGANIZATION

During the reporting period, the Applied Mathematics Division underwent a reorganization. Table I shows the division before reorganization and Table II shows the divisional organization as it is presently constituted.

APPLIED MATHEMATICS DIVISION

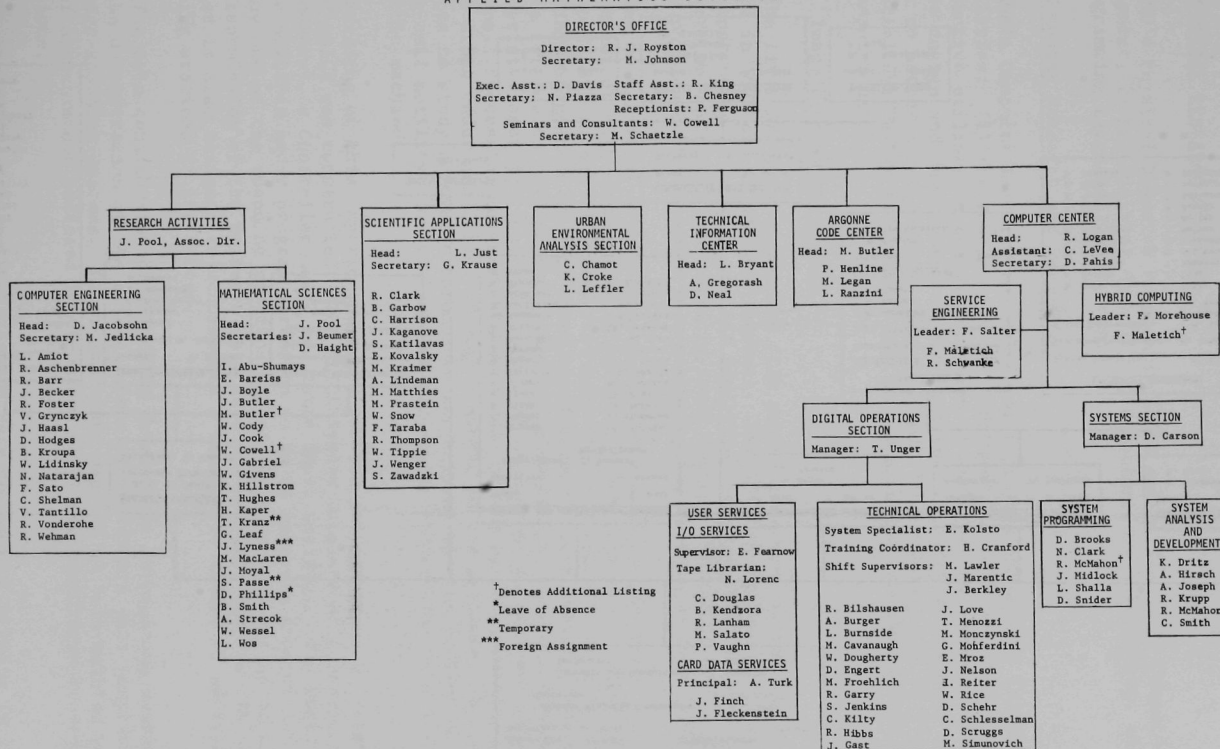
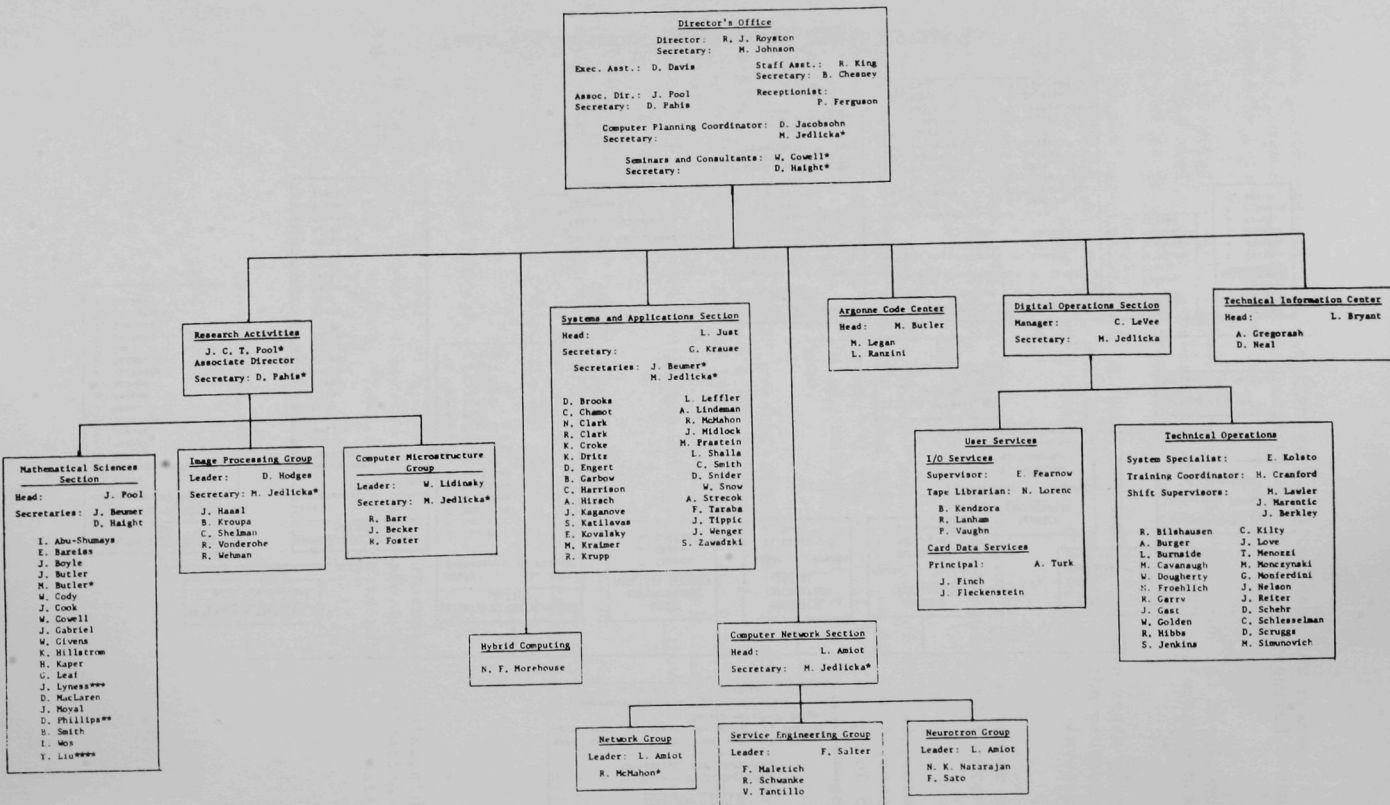


Table I. Division Organization (March 1972)

APPLIED MATHEMATICS DIVISION



* Denotes additional listing
 ** Leave of absence
 *** Foreign Assignment
 **** Temporary

Revised 8/9/72

Table II. Division Organization (June 30, 1972)

3.0 PHYSICAL RESEARCH PROGRAM

AMD's Physical Research Program includes activities in 1) Computer development, 2) Mathematical Physics, 3) Computational Mathematics, and 4) Programming Languages and Systems.

3.1 Computer Research and Development

AMD's Computer Research and Development program emphasizes the following capabilities: (1) the development of techniques for evaluations that lead to effective utilization and exploitation of contemporary computer hardware, (2) the design and development of new hardware and hardware-oriented techniques to better solve current problems, and (3) the design and development of special systems to bring novel and unique problems into the domain of the computer art.

3.1.1 Image Processing (ALICE)

The first AMD general-purpose film scanning system, called CHLOE, was retired in 1970 due to its obsolescence. Two special-purpose devices were then constructed to provide special facilities not available with CHLOE. They were an emulsion plate particle track counter (PAULETTE) and a high-energy physics bubble chamber film measuring and scanning system (POLLY).

The main initial application of the CHLOE scanning equipment was in the measurement of high-energy physics particle track film data. CHLOE also gave good performance on a number of other photointerpretation problems, including measurement of high-speed oscilloscope traces, metal fragmentation studies for reactor safety heat transfer calculations, bone characterization, fingerprint classification, and ecological studies of desert weed growth patterns. Successful measurements were made of the evaporation rate of liquid drops under conditions of high temperature and pressure. Research projects to study automatic chromosome karyotyping and the problem of quantifying living cell motility from analysis of time-lapse photographs were also begun with this machine.

Building on this experience, a new general-purpose image processing system called ALICE was constructed. The ALICE System consists of a PDP-10 computer (32K memory), a Controller unit, and three input stations. The Controller can be switched under program direction so as to generate control information for any one of the scanning stations and at the same time set up data paths for transmission of the measured data into the computer memory. The Controller is also designed to accommodate a reasonable number of additional scanning stations in the future.

The main contribution of the CHLOE development to scanning system design was the demonstration of the effectiveness of coordinate data compression in image-scanning systems. Other important aspects of this machine were the use of asynchronous buffered input-output (I/O) and overlapped scanner control functions.

In the POLLY development it became very convenient to think in terms of a human operator on-line to the scanning and measuring system who was

available to the machine whenever some higher-level (usually global) pattern recognition decision had to be made. All questions were eventually asked of the human operator in a graphical manner and were answered in a similar way by the operator. All of these hardware techniques have been incorporated into the ALICE system.

The ALICE system carries this asynchronous control philosophy several steps further by incorporating more computational power into the scanner controller. The controller is designed as a second processor on the PDP-10 memory and is such that the scanning pattern can be virtually any subset of the basic 4096 x 4096-point raster that can be described in terms of areas, lines, or points. The ALICE controller is independent of the image source, so that besides conventional film digitizers the system can accept data from image sources such as a conventional optical microscope or a scanning electron microscope.

Another new feature of the ALICE system is the use of digital logic to compute the combined pincushion and dynamic focus correction, a function which was done by analog circuitry in CHLOE. The digital corrector yields more repeatable results and is easier to adjust when attaching different scanning input stations.

The controller and the first 16- and 35-mm film digitizing station have been operational for about two years.

A second cathode-ray-tube digitizer station for 35mm film has been completed. The design of this station emphasized the reduction of electronic noise in the light measuring system and the minimization of scattered light contributions, these being the most important factors limiting accurate and reproducible film density measurements.

A significant reduction in the noise level was achieved by incorporating an integrating circuit immediately at the photomultiplier output, so that the signal fed to the A-to-D converter is derived from integration of the photomultiplier pulse over essentially the entire bright-up time of the light signal. Other noise in the form of occasionally occurring large electrical spikes was reduced by careful selection of photomultiplier tubes.

Scattered light contributions were reduced by paying attention to the geometry and internal reflectivity of the light path and by constructing between the imaging lens and the film a movable slit which travels across the film plane in synchronization with the spot deflection waveforms.

Preliminary experience with the second film station (Station 1) has shown consistently better density measurements relative to Station 0, although the precise degree of improvement has not yet been measured.

A film output device has been added to the system so that graphic hard copy output can be obtained in the form of 35mm sprocketed film negatives. This unit is built around a 35mm camera with electrical film advance and a high precision CRT which is slaved to the existing display station.

The technique of image data compression by shape construction or binning was developed and has proven its worth in most of the image-processing applications that have been undertaken. This technique has the desirable property of allowing the writing of more general-purpose computer programs, in which parameters are the variables, rather than requiring completely new programs for each application. The use of moments and moment invariants as shape classifiers has proved to be useful in a variety of problems, including the chromosome karyotyping project.

The task of programming ALICE to take over work formerly done on CHLOE has been completed. In the course of this work, a scanner service module and Fortran driver were added to the ALICE monitor system. The monitor system supplied with the control computer has a modular structure that permits new I/O devices to be connected by writing appropriate device service modules.

The ALICE service module allows programming of scanning operations at assembly level without explicit attention to interrupts or input buffer space allocation. A Fortran-callable "driver" program communicates with the service routine so that all scanner functions can be programmed in Fortran.

To facilitate future research with the ALICE system, several useful features have been added to the Monitor. These include asynchronous teletype I/O, DECTape subfile capability, and the ability to respond to interrupts from the arithmetic processor. An approximate round object signature filter has been used successfully in a production program for the counting of nerve fibers in photographs of optic nerve sections from mice, monkeys, and humans.

3.1.2 Computer Systems Performance Measurement and Analysis (Neurotron Monitor)

Previous use of commercially available hardware monitors demonstrated the need to obtain information directly at a more primitive level, in greater quantity, at higher bandwidths, and with more convenient and condensed output facilities. To this end, the Neurotron monitor system has been developed and is available for use at Argonne National Laboratory to achieve a more creditable means of system measurement and evaluation.

This monitor is unique in its ability to interact with the monitoring processes and to provide analysis and display of current measurements. The monitor development has aided in solving the problem of information loss due to sampling while reducing the data collection rates and raw data storage and processing requirements. The Neurotron monitor provides for interaction by the operator or program with the data accumulation, analysis, and display processes. This interactive monitor is based around a minicomputer, storage display, tape control, and highly specialized computer-controlled logic and data accumulation hardware.

An interrupt-driven, multiprogram priority-oriented operating system has been written and tested for use in this interactive and multiprogramming environment. This system provides for the concurrent operation of display, tape control, operator requests, data acquisition and analysis, and program and hardware control.

The dynamic capabilities of the Neurotron have necessitated the development of data acquisition programs, display programs, and buffering techniques not normally used in other monitors. The wide bandwidth of incoming data, hardware sampling rates, and the nature of the data collection equipment place time dependencies on the acquisition and analysis programs. A few general acquisition programs that can be applied over a spectrum of problems are now operating. The on-line graphics facility has proven valuable in preliminary data analysis and probing, saving considerable time in monitor setup.

The interactive display has provided a means of pre-acquisition probe adjustment, of judging the reasonableness of the on-line data acquisition and reduction programs, of obtaining "snapshots" of the performance statistics during data collection, and of providing information to inquiries by means of messages, histograms, bar charts, time plots, etc.

The analysis of complex systems requires nontrivial knowledge of its subsystem performance. Our monitoring efforts have provided information in several areas, including

- insight into the operation of complex subsystems,
- development of monitoring techniques,
- identification and sensitivity of subsystem parameters,
- generation and/or verification of subsystem models, and
- measures of subsystem capacity requirements.

Monitoring results have shown the disparity of resource utilization between single stream batch processing (similar to rapid response control systems), multiprogramming (also typical of time-shared terminal systems) and "large" production code execution. The measurements point up the difficulties in obtaining a balance in CPU, memory, and peripheral performance. The design of future parallel system organizations should attack this balancing problem.

Additional monitoring has provided a preliminary analysis of benchmark programs and utilization of current system resources during execution of these Laboratory representative programs. This work has affected current use and future design planning for optimum system performance.

At least one commercial performance measurement company is now considering reproducing the Neurotron. Other companies have shown substantial interest in its development.

3.1.3 Microstructure and Computer Graphics (MIRAGE)

The Argonne Interactive Display (AID) system was developed to provide computer-generated low-cost standard television images in full color with no flicker. The system consists of an IBM 1130 computer, a refresh disk, a display controller, and several raster scan displays. A graphics programming language was developed for the system and the AID system has been incorporated into the MIRAGE system.

MIRAGE is an interactive microprogrammable graphics system which utilizes raster scan display techniques to provide full-color computer-generated pictures. It consists of a general-purpose computer, an expandable microprogrammable display processor, and a variety of peripherals including a 7-track tape unit, a quality high-speed hard copy device, a display controller, and two display monitors. A meta-assembler called ARGOT, running on the System/360, is its main software support.

The present system will operate in a "stand-alone" mode. In this capacity it will be capable of such things as reorganization and modification of input data, generation of displays and hard copy, handling of user interactions, and creation of additions to input tapes for use in further processing on other computers.

MIRAGE is designed to handle a wide variety of display list formats. In addition, the processor has instructions that augment the instruction set of the general-purpose machine. Examples of these are automatic stack manipulations, various list-processing instructions including tracing, masking, and moving operations, and automatic character string identification and generation.

The computer and the display processor operate asynchronously with respect to each other from common memory. The expandability and microprogrammability of the display processor provide a means of easily modifying its architecture, machine instruction set, and organization.

ARGOT, which provides the main software support for MIRAGE, is a meta-assembler that provides automatic library facilities and extensive macro-processing capabilities to developers of programs for small object computers. ARGOT is written in PL/I for execution on the IBM System/360; it makes the speed, memory, and I/O facilities of the 360 useful to the smaller computer user. Because of ARGOT's structure, little effort is required to establish versions for other object computers.

The initial version of ARGOT assembles and link-edits programs for the following computers:

- Digital Equipment Corporation PDP-7, PDP-9, PDP-11, and PDP-15;
- Control Data Corporation 160-A;
- Varian Associates 620/i; and
- the MIRAGE microcontrol and graphic controllers.

To assist in the development of MIRAGE, a wirewrap and debugging program was written. The program provided input to allow the processing of a wide variety of wirewrap circuit boards and integrated circuit types, minimum wire length analysis, significant hardware design diagnostics, and output for direct use by (commercially available) automatic wirewrap machine tools. Many man hours of generating wire lists were saved through the utilization of this program.

Other ANL divisions, namely Electronics and EBR-II, are planning to use the wirewrap and debugging program as an aid in designing their systems.

3.1.4 Benchmarks

A well-controlled representative job data base is essential for system performance study and evaluation. The development of such a data base, or benchmark collection, for the ANL environment has been carried out in two separate but related sections. The first consists of problems representative of and essential to ANL's discipline-oriented research programs and reactor development project; the second consists of a sample job-stream simulating the Laboratory's computing workload.

The collection requires continual review and modification to ensure its timeliness and adequacy. The benchmark collection includes 24 applications problems representative of the Laboratory's discipline-oriented research programs and reactor projects, four applications problems contributed by the National Accelerator Laboratory as representing their requirements, and a 60-job model job stream developed from a sampling of our computing workload.

This benchmark collection was distributed to vendors participating in a Laboratory computer acquisition study, and an experiment designed to use the collection to measure the performance of the proposed computer systems was undertaken in conjunction with these vendor personnel. Control Data Corporation converted and executed 24 of the 28 benchmark application problems and 57 of the 60 jobs in the job-stream benchmark on their CDC 7600 system; IBM executed all 28 of the applications problems and ran all of the job-stream benchmark on several configurations with their System 360 Model 195. A detailed analysis of these runs has been completed, and a document summarizing the significance of the results obtained has been distributed to the ANL Computer Selection Committee.

3.2 Mathematical Physics

Research activities in the area of Mathematical Physics are directed primarily towards the development and analysis of procedures for the numerical solution of the equations of neutron transport and diffusion, hydrodynamics and magneto-hydrodynamics, and magnetism and electromagnetism. These equations may appear in differential, integral or integro-differential form, and may be linear or non-linear, depending on the model employed for the description of the physical phenomenon under consideration. Their solutions are involved in many research and engineering programs of importance to AEC missions, for example, in the areas of fission and fusion reactor design, reactor safety analysis, and particle accelerator design.

The research activities are pursued not only by investigating specific computational procedures, but also by studying the mathematical foundations underlying the physical models. An understanding of these foundations is a necessary condition for the successful development of reliable and efficient computational procedures.

3.2.1 Application of Finite-Element Techniques to the Solution of the Neutron Transport and Diffusion Equations

The neutron transport and diffusion equations form the basis for all deterministic mathematical models of reactor systems. In the continuing study of the physics, design, and safety of fast breeder reactors, an

increasing demand for more exact knowledge of the neutron distribution inside the reactor is inevitable. Thus, the efficiency of methods for the numerical solution of the neutron transport and diffusion equations has become a factor of major importance. All operational methods developed so far are characterized by an approach based on low-order approximation procedures coupled with iterative solution techniques. Their application to three-dimensional reactor problems is not feasible.

This study, therefore, has departed from the traditional approach in order to develop and analyze a particular class of high-order approximation procedures based on the use of variational principles and subspaces generated by finite element techniques. In a finite element technique, the domain of definition of the unknown function is considered as the union of a finite number of subdomains of elementary shape (triangles, quadrilaterals, tetrahedra, etc.); the approximating function is constructed in such a way that in each subdomain it is equal to a polynomial function which is characterized entirely in terms of the data pertaining to the subdomain. The use of finite element techniques introduces a symmetric band structure and reduces the size of the resulting system of algebraic equations, so that a direct inversion technique may be realistic.

Since current studies for liquid metal fast breeder reactors are based on core designs involving subassemblies which are hexagonal prisms arranged in concentric rings, this project seeks solution techniques for the one-group transport and diffusion equations in two-dimensional hexagonal geometries. In accordance with the standard fast reactor core designs, material properties are allowed to vary on a subassembly basis.

Considerable progress has been made in the part of this research effort which is related to the neutron diffusion equation. The results can be summarized as follows.

- The use of high order finite element methods offers a significant advancement in computational capability for the numerical solution of the neutron diffusion equation on a broad class of fast reactor configurations.
- With high order approximation procedures based on finite element methods it is possible to obtain, at a reasonable cost, solutions to the neutron diffusion equation which are sufficiently accurate that any errors can be attributed to either the diffusion theory approximation or other approximations in the reactor model, rather than to the numerical approximation procedure.

These results were obtained using a prototype High-Order Diffusion program (HOD) developed as part of this project. Solutions obtained from HOD were compared to those obtained using DARC2D, the two-dimensional diffusion module of the Argonne Reactor Computation (ARC) System, which is based on the use of low-order finite difference approximations. The comparisons were performed for three different types of reactor configurations: a simple two-zone configuration with two energy groups, a multizone configuration (1,000 MWe LMFBR mockup) with four energy groups, and a loosely coupled configuration with two energy groups.

The timing comparisons were based on the execution times for a k_{eff} -calculation with a prescribed accuracy. Execution time ratios on the two-zone and loosely coupled configurations ranged in value from twelve to over fifty in favor of HOD, and on the LMFBR mockup the same accuracy in k_{eff} was achieved approximately twenty times faster with HOD than with DARC2D, while using thirty percent less storage. Furthermore, solutions obtained with the finite element method provided flux inventories whose accuracies were comparable to the accuracy of k_{eff} . Detailed results of this study have been reported in ANL-7925.

For the neutron transport equation the function space to which the solution belongs and the properties of the solution have been identified, and the formulation of a Galerkin-type approximation procedure has been completed (see Applied Mathematics Division Technical Memorandum TM-219). On the basis of this formulation, the development of a research computer program for the numerical solution of the neutron transport equation on two-dimensional reactor configurations has been started.

3.2.2 Analytic Transport Theory

Greater understanding of the structure of the transport operator in three space dimensions will yield results which will be significant for predicting, explaining and possibly resolving difficulties in computational methods. The transport operator is not self-adjoint; consequently, conventional spectral theory is not applicable. Although no spectral theory is yet available for the transport operator in three dimensions, a spectral resolution for the case of one space dimension has been developed.

Additional results have been obtained in connection with the one-to-one transformation that maps the three-dimensional transport equation into an ultrahyperbolic partial differential equation. The method of characteristics was used to prove the existence of elementary solutions for the partial differential equation. Further, these solutions have been shown to be solutions of a mixed boundary value problem (Robin's problem) of potential theory. Therefore, the elementary solutions of the transport equations (the normal modes) are transformations of solutions of a potential theory problem. This established a direct connection between transport theory and potential theory.

Since surface harmonics are encountered frequently in multidimensional transport problems, these functions have been derived in a simple, novel, and mathematically rigorous way, and some new relations and properties have been proved. In particular, this new approach greatly simplifies some cumbersome methods of finding the inverse of the scattering operator.

Symmetry properties of the inverse generalized three-fold two-sided Laplace transform and analytic continuation have been used to show how to determine the expansion coefficients for the normal mode representation of the angular distribution of neutrons in an infinite source-free medium.

An unsolved problem in the normal mode approach for three dimensions (as used during the past decade) has been the representation of singularities in the space variables and thus the failure to account for point sources.

A new type of elementary solution which allows for such singularities has been recently introduced. These new solutions will be denoted as *normal modes of the second kind*.

New analytic solutions of the transport equation, including polyharmonics and double harmonics have also been introduced in an attempt to provide improved approximations to the actual neutron distributions in finite domains. A linear combination of such exact solutions can be expected to yield good approximations when used as trial functions in variational methods for solving the general transport equation with region-wise constant parameters.

3.2.3 Analytic Transport Theory and Numerical Investigations

In actual reactors with many components, the cross-sections, source terms, etc., are usually discontinuous across interfaces. The neutron flux and angular distribution, in fact, have logarithmic singularities of their derivatives near material interfaces and vacuum boundaries. Thus, it is expected that the accuracy of computational methods for the numerical solution of the transport equation (and mainly those based on higher order approximations) depends critically on how well one can account for the exact behavior near boundaries, edges and corners. G. Fix has provided evidence in an analogous situation for the diffusion equation.

The finite element method in slab geometry is being studied to evaluate the effect of including singular elements that approximate the local behavior near boundaries. This project supplements other efforts in the Applied Mathematics Division to develop finite element approximations for the solution of neutron transport and diffusion problems in two and three space dimensions. It assesses the extent to which the exact behavior of the neutron concentration near interfaces, edges and corners should be sought and incorporated in higher order computational methods.

In implementing the finite element approach for one dimensional transport the need arose for low-order Gauss-Christoffel quadrature for numerical integration. This led to development of a Fortran IV program capable of generating, simply and cheaply, these needed low-order ($n=1, \dots, 16$) Gaussian quadrature formulas. This program is applicable in general whenever the weight function is sufficiently smooth and has known moments. The program has been documented together with two illustrative examples, including an application for the numerical integration of functions with logarithmic singularities.

As an integral part of the numerical work, an initial version of an efficient and flexible computer program for cubic spline interpolation in one dimension has also been developed. Most of the cubic spline programs already available either restrict the boundary conditions to knowledge of the first derivative at both end points, or require the second derivatives to vanish at these points. The program mentioned here removes these restrictions. The advantage is demonstrated for the extreme case of interpolating the function $x \log(1/x)$ which is characteristic of the neutron flux near an interface and which has singularities in all its derivatives at $x = 0$.

3.2.4 Stochastic Aspects of Reactor Theory

Significant advances in numerical analysis of the neutron transport and diffusion equations--for example, advances which lead to reductions in computation time--can be expected; however, these mathematical models have been around for a long time, so qualitative as opposed to such quantitative advances will be increasingly rare.

Any new classes of models will presumably have to be derived from the fundamental stochastic model, the Markov process, from which only first moments are selected for analysis by transport/diffusion theory. Higher moments have additional information to give about the reactor, information about statistical fluctuations which will be more important in the fast breeder program than it was for thermal reactors.

Statistical mechanics provides no rigorous derivation of the general nonlinear transport equation for the kinetic theory of gases. But the special statistical mechanics of the "neutron gas" is greatly simplified because neutron-neutron scattering is negligible. Once $d\mu/dt = A\mu$ is rigorously defined the foundations of the entire theory can be made rigorous because the marginal projection of μ down to the neutron flux takes that equation directly into the neutron transport equation in its usual initial-value formulation. For example, the nature of approach to equilibrium, a mathematical mystery in the general kinetic theory of gases, is here nicely handled by the Perron-Frobenius theory of morphisms of Banach lattices.

The Perron-Frobenius theory was first introduced into reactor theory in an existence and uniqueness theorem for the outer iteration computation scheme which initiates evolution of the flux. The existence and uniqueness theorem for the underlying Markov process has been based on the integral equation extensively studied by J. E. Moyal, rather than the initial-value differential equation. Now that theorem has been proven in the initial-value formulation.

In the case of sub-critical assemblies there is, alongside the above theory of time-dependent behavior of the probability distribution μ , a theory of time-independent behavior of generalized states which, unlike probability distributions, cannot be normalized. Such assemblies can be analyzed by their scattering properties as modeled in either of these two theories: the scattering of a neutron pulse (time-dependent) or the scattering of a neutron beam (time-independent). As in quantum mechanics, there is an "S-matrix" theory which unifies these two approaches. The fundamental theorem here is existence of the limit

$$\lim_{t \rightarrow \infty} e^{-A_0 t} e^{2At} e^{-A_0 t},$$

which is supposed to converge to the "S-matrix." ($e^{A_0 t}$ is the group of transformations which would govern evolution of the Markov process if all cross-sections were set to zero.) This theorem has been proven.

Dynkin's theory of weak infinitesimal generators, which does not require the adjoint space necessarily to consist of continuous functions, provided the needed generalization of Feller's theory. Difficulties caused by unboundedness of the scattering perturbation (even when cross-sections are bounded, restriction of the scattering perturbation to n -particle space admits only n times that bound, and n goes to infinity) were surmounted by a perturbation expansion each term of which is bounded on a suitable domain. This expansion has been shown to actually represent a semigroup e^{At} with the desired infinitesimal generator.

3.2.5 Population Processes

One of the major experimental methods for determining the means and variances of the durations of the phases in the life-cycle of a biological cell is the determination of the fraction-of-labeled-mitoses (FLM) function. Various ad hoc methods for estimating the means and variances from the FLM-function have been used in the past, but what has been needed is a systematic method of analyzing FLM-data by computer.

Using previously developed mathematical analysis, a computer program has been developed which takes a set of FLM-data and from it estimates the means and variances of the durations of the first three phases of the cell-cycle (the duration of mitosis is assumed known by other means). Monte-Carlo methods for generating theoretical FLM-curves have also been developed.

The distribution of the time to extinction of a population process where the increments in population size in successive time intervals form a Markov chain has been investigated.

The theory of branching processes (on which the mathematical analysis of the FLM-function is based) can also be used to analyze other experimental techniques which are used in the study of the cell-cycle, e.g. continuous labelling experiments. Branching processes in which the distribution of the number of offspring per parent is subject to control depending on the size of the population are of interest in many scientific areas. In particular, the population of neutrons in a reactor as a function of time is such a process, the control being supplied by the insertion and withdrawal of control rods.

3.2.6 Mathematical Foundations of Quantum Physics

The mathematical foundations of quantum physics are being investigated for systems with infinitely many degrees of freedom. Emphasis is upon the role of group theoretic and probabilistic concepts.

The concept of a "system of imprimitivity" introduced by G. Mackey has served to clarify the application of group theory to relativistic quantum mechanics. It has been suggested by Mackey that this concept could be usefully introduced in the area of quantum field theory.

A research investigation on the relation between the general theory of number operators and the theory of stochastic population processes, has been completed. An account of this work, entitled "Particle Population and

Number Operators in Quantum Theory," appears in *Advances in Applied Probability*. On the basis of the results of our investigations, study of the application of the theory of population processes to the statistical mechanics of infinite systems is presently being undertaken by D. Kastler and coworkers at the University of Marseilles (France).

3.2.7 Number Operators and Population Processes

Quantum field theory provides the researcher with a set of rules of supposedly unlimited generality. The theory can be applied to any system to forecast how classical concepts have to be modified and how quantum features arise in the system under consideration. Consequently, quantum field theory can lead to an understanding of the fundamental features of matter. A basic feature of quantum field theories is the existence, in certain situations, of an interpretation of the observables of the theory in terms of particles.

Using methods taken from the theory of stochastic population processes, the joint distribution of numbers of particles in various states in soluble examples of field theory have been calculated. In the case of a scalar field with sources, for example, where an explicit expression for the S-matrix is available, one can calculate the exact generating function for the final joint distribution of particle numbers n_k in various momentum states k , conditional on any initial numbers at $t \rightarrow -\infty$ (in the special case where the initial state is a vacuum, the final state is a Poisson process).

It is expected that these techniques will be useful in problems involving a quantized field coupled to a system with a finite number of degrees of freedom (e.g. in laser or in solid state theories).

3.2.8 Symmetrization

Perturbation theory starts with a symmetric object and considers the effect of asymmetrizing influences. "Symmetrization" is proposed as the name of a reverse theory. Starting from an unsymmetric object, an asymmetry is removed by averaging over the symmetry group. Then such asymmetries as remain must be the result of influences not yet averaged out, and the search for such influences can be narrowed accordingly. Present studies concern the symmetrization of stochastic processes.

The concept was suggested by a project in Argonne's Biological and Medical Research Division to study the removal of all orientation dependence from environmental influence (e.g., gravitation, electromagnetic radiation) on the growth of a biological organism. Then deviations from spherical symmetry would presumably be due to intrinsic asymmetries in the organism itself. This project, funded by NASA, looks forward to the day when plants and even human embryos will be growing in the weightless environment of outer space.

Another application was suggested by the need for a good random number generator for Monte Carlo calculations. (Algorithmic generators are being abandoned because of asymmetries uncovered at Boeing Scientific Research Laboratory.) A generator is "good" if and only if it produces a probability distribution invariant under its defining symmetry group.

A symmetrizing pattern of motions (an ergodic path in the rotation group) was found. It was implemented for the Biological and Medical Research Division by a device constructed in the Electronics Division.

The device, now completely in the hands of the Biological and Medical Research Division, is successfully producing biological specimens.

A random number generator was purchased, but statistical tests immediately showed disappointing asymmetries (biases, correlations, non-stationarity, etc.) and it was decided to go to a more fundamental scheme rather than try to symmetrize the output algorithmically.

N. Frigerio of the Biological and Medical Research Division constructed a random number generator based on radioactive decay. It has been connected to our hybrid computer. A tape of random numbers has been produced for use in any Monte Carlo calculation.

The randomness derives from the high degree of symmetry (very large group) of the quantum field theoretic "vacuum," whose fluctuations stimulate radioactive decay. So, as we remove asymmetries introduced by the measuring device, we will be testing for asymmetries in the vacuum state, presence of which would contradict modern physical theory as its deepest level.

Both projects were done in close collaboration with needs of other divisions, who contributed financial support to AMD.

3.2.9 Quantum Theory of Measurements and Probability Theorem

The "quantum logic approach" to the mathematical aspects of the foundations of quantum physics provides a mathematical framework for formulating and investigating mathematical constructs corresponding to physical concepts. Simultaneous observability, real-valued observables, superselection rules, hidden variables, and symmetry are examples of physical concepts which have been treated. However, few new physical ideas have been studied using the quantum logic approach since the original work of Birkhoff and von Neumann. In particular, the most controversial question throughout the history of quantum mechanics, the so-called "projection postulate," has received little attention.

An axiomatic structure generalizing both von Neumann's Hilbert space model of non-relativistic quantum mechanics and the conventional measure theoretic model of probability theory has been formulated. The projection postulate of the quantum theory of measurements was found to be analogous to conditional probability. The introduction of concepts associated with the projection postulate promises to yield new insights into the mathematical structure of quantum mechanics and its relation to probability theory.

3.2.10 Cascade Processes

In a nucleon-meson cascade, a high energy primary particle interacts with a nucleus to produce a number of energetic secondary pions and nucleons, each of which may generate further cascade particles. The iterative method

developed for the ionization cascade was combined with the "pion-link" method of Wayland and Yodh (Physics Department, University of Maryland) to calculate the lateral distribution of such a cascade in the atmosphere. The method compares favorably with Monte Carlo techniques as to both accuracy and computational speed.

3.2.11 Computational Aspects of Non-Linear Classical Fields

Many research and engineering programs of importance to AEC missions require efficient computer solution of classical field problems. Examples in the areas of hydrodynamics, non-linear magnetics, and electromagnetic field calculations are numerous.

Computationally difficult problems in hydrodynamics are involved in such important areas as reactor safety (e.g., disassembly codes) and coolant (liquid metal) flow analysis in reactors.

Problems in non-linear magnetics are involved in the economical and efficient design of particle accelerators and in the development of magnetohydrodynamic generators (MHD) and controlled thermonuclear reactors (CTR) as energy sources. Particularly severe problems of this type will arise as the CTR research program phases into efforts to design fusion reactor systems.

The first task undertaken was an attempt to improve an existing magneto-statics computer program (TRIM) in the direction of producing more accurate calculated results in less computer running time. This code is used locally for magnet design problems by three ANL divisions (the Chemistry, Accelerator, and Physics Divisions) and by the National Accelerator Laboratory.

TRIM is designed to solve two-dimensional problems; it makes use of an essentially arbitrary triangulation of the field region, making it easy to fit the complicated component shapes often encountered in magnet problems. The overall conception and design of the code were very good; however, it suffered from slow convergence behavior and sometimes inaccurate determination of field values from the computed vector potentials.

The convergence behavior of TRIM has been improved, and thereby the running time on some typical problems has been decreased to as little as one-tenth of the previous time.

Some work has also been done on the general problem (the "editing" problem) of computing field values from the potentials, which are usually the quantities actually computed in iterative programs of this type. An existing harmonic editing routine was improved to give more accurate results near interfaces. Most of the programming for a PL/I module INTERP, based on a new mathematical method, has been completed.

3.2.12 Electron Optics and Electron Beam Technology

The calculation of electron lens aberrations calls for the solution of interesting and unconventional types of computational problems that are likely to have other applications. The subject is basically an application of classical particle dynamics; areas of mathematics involved are the solution

of ordinary differential (trajectory) equations and the solution of electromagnetic field problems. This activity is being pursued with the aim of producing new results in electron optics which can be utilized by scientists and engineers in this important field.

The first major result of this research was the design of a field-emission electron gun with a low value of spherical aberration. This gun is now in use at several scientific institutions and is also being commercially marketed. The apparatus used by A. V. Crewe in viewing single atoms utilized a gun of this design.

Subsequent investigations into high-frequency electron optics led to a demonstration of the feasibility of constructing high-frequency electron lenses with no spherical aberration.

3.2.13 Fluid Dynamics - Numerical Simulation

Several important practical situations concerning the dynamics of fluids are being studied. The most frequently used method of solution involves the use of fairly large computer calculations to solve the relevant partial differential equations or to analyze field data.

Work is continuing on three problems concerning the dynamics of the upper ocean. The physical questions common to these studies are the vertical energy transfer and/or the crucial interaction of gravity with the variable fluid density.

Numerical experiments are being conducted in a study of the sea surface temperature and the heat transfer processes across an air-water interface. Correct evaluation of these small-scale processes is important in the calculation of the mass-energy balance between the atmosphere and natural bodies of water and the evaluation of the effect of large bodies of water on weather movements and climatology.

Specific physical phenomena for which studies have been completed include

- a) convection currents in water where the surface is cooled by evaporation and infra-red radiation (the surface is assumed to be stress-free and perfectly flat);
- b) forced convection of heat at a surface on which an internal gravity wave impinges (density effects on the motion are neglected); and
- c) forced convection of heat in the surface thermal "skin layer" in the presence of irrotational surface waves.

A computer program for solving the Navier-Stokes equations governing the two-dimensional flow of an incompressible fluid with a free surface has been developed. The program allows for an arbitrary density stratification and a mixed wake with initial vertical momentum. Certain surface effects, chiefly radiation and evaporation, that are difficult to compute within this program are handled by coupling to the separate program written for problem b.

Calculations performed on the collapsing wake problem have yielded solutions that compare well with the results of experiments at Hydronautics, Inc. and experiments by Schooley at NRL. One interesting result obtained during the past year is the observation of strong coupling between thermocline waves and a wake collapsing near the thermocline. At present, calculations are being performed on the collapse of a wake in a number of realistic density stratifications chosen from the Oceanographic Atlas. In the future, a number of calculations using newly measured ocean density gradients are to be performed as an aid in interpreting field experiments.

3.3 Computational Mathematics

3.3.1 Linear Algebra Over an Integral Domain

Solutions of a linear system of equations, given enough time, can always be produced as rational expressions of the input data. The multistep Gaussian elimination method (reported in ANL-7213) has proved very successful for the problem of symbolic matrix inversion.

The work done at Argonne consisted of generalizing a theorem by Sylvester (Sylvester's Identity) and applying the generalization to solve systems of linear equations. Because of the similarity to a well-known method, the resulting process is called Multistep Gaussian Elimination. It has the following properties.

- The results are equivalent to the results obtained by Cramer's rule.
- The expressions that are obtained during evaluation of the corresponding algorithm are the "simplest" possible for a general matrix.
- The efficiency is at least equivalent to any known method, and in many cases is much better.

An algorithm, "Integer-Preserving Gaussian Elimination," has been coded at Argonne for both the CDC 3600 and the IBM 360/75. The algorithm uses the two-step method and provides for the numerical solutions of linear systems in double precision or, optionally, in integer arithmetic. The code has also been adapted, by the use of FORMAC, so as to permit integer arithmetic with numbers of up to 2000 digits on the IBM 360/75. The algorithm for the two-step Gaussian Elimination Method with multivariate polynomials as matrix elements has been coded at Harvard University and by IBM for calculating the generating functions of flow graphs. The method is also being tested at Westinghouse in connection with the solution of boundary value problems for partial differential equations by the finite element method.

Since many applications in physics, statistics, and algebra require the inversion of Toeplitz or Hankel matrices, a method was developed that permits the direct solution of these problems, requiring only of the order of n^2 multiplications instead of the n^3 multiplications required by Gaussian Elimination. This method has been expanded to permit operation over an integer domain. In particular, algorithms based on this method should be useful

in calculating the exact or the symbolic inverses of matrices that contain Toeplitz matrices as submatrices.

A prototype matrix inversion routine using the multistep method and the Ehrman multiple-precision floating point arithmetic package has been coded and tested.

A thorough comparative analysis of the two-step elimination and congruence technique methods was conducted. In the course of these investigations a new and considerably more efficient termination criterion for the congruence technique was discovered.

A unifying theory from which follows the above-mentioned multistep Gaussian elimination and also the integer-preserving algorithm for the inversion of Toeplitz matrices has been developed. In investigating congruences over the ring of polynomials the equivalence of congruence techniques and polynomial interpolation was shown; in particular, the equivalence of the Chinese remainder theorem and the Lagrange interpolation formula and the equivalence of the mixed radix representation and Newton's fundamental formula were displayed. Furthermore, it was shown that for the integer-preserving algorithms a special "short" division exists.

Matrix inversion over an integral domain facilitates the work of the numerical analyst, as opposed to inversion over, say, the field $R^{\#}$ of reals. Other uses for such methods are found in integer linear programming, in solving linear diophantine equations, in the calculation of matrix invariants and in problems of number theory.

Various methods of handling matrix problems over commutative rings are discussed by Bareiss (1972). These methods are, briefly,

- multistep methods for general multivariate polynomials; $P[x_1, x_2, \dots, x_r]$ of degree d over some field f in the indeterminants x_1, \dots, x_r (including the field itself when $r = 0$, and $P[x]$ when $r = 1$);
- division-free methods and row-wise simultaneous reduction by a greatest common divisor;
- interpolation methods; and
- congruential methods.

Of these, the multistep methods are shown to be more efficient than the others in the sense that these methods require fewer single-precision multiplications. Among the multistep methods themselves, the two-step method is shown to be about fifty percent more efficient than the one-step method.

We have reviewed and unified the work done in these areas in the past decade and the results have been published. ("Fast Algorithms and Fast Arithmetic in Linear Algebra," Argonne National Laboratory Report ANL-7897). Also, the problem of optimizing the general multistep elimination method has been investigated. It was possible to derive a symbol matrix from which the general fixed l -step optimal algorithms can be derived in an elegant form. These

ℓ -step methods have an eighty percent efficiency advantage over the one-step method. (The variable step method was also investigated, but the theoretical predictions showed gains in efficiency of less than five percent over the optimal fixed step method.) Six different codes, representing fixed two-step, three-step, and optimal ℓ -step algorithms for different types of problems, were written. The theoretical predictions of efficiency and optimum configurations were tested on matrices of order up to one hundred over the ring of integers, and the interesting fact that the step configuration is not unique (non-convexity theorem) for rectangular matrices was confirmed.

3.3.2 Matrix Mappings

The four matrix mappings studied arise naturally from their relations to one of them, namely, Lyapunov's 1892 differentiation mapping of "energy-like" positive definite quadratic forms on n variables depending on a system of n ordinary linear differential equations $\dot{x} = Ax$, the solution of which is required to be stable. For a quadratic form $Q = x^T G x$, the derivative is another form $\dot{Q} = x^T H x$. The Lyapunov mapping $G \rightarrow H = GA + A^T G$ is naturally extended to all symmetric matrices. Unfortunately for the convenient use of Lyapunov's method for establishing stability, it is the inverse mapping $H \rightarrow G$ which is required.

Better theoretical or numerical techniques for obtaining the inverse mapping could be used in such areas as the design of control mechanisms.

In searching for a basis for the linear vector space of symmetric matrices which would facilitate inversion of $G \rightarrow H$, it was observed (for the fundamental case when A determines a cyclic mapping) that a mapping of symmetric to skewsymmetric matrices played a key role. This resulted in a useful new connection between the Lyapunov and Hurwitz stability criteria. The structure (at the level of invariant factors) of a general matrix was then applied to obtain new structural facts about the Lyapunov mapping determined by the given matrix. A three index tensor with invariant properties was then discovered. Known results on the possibility of replacing the eigensystem problem for a general matrix by that for a symmetric pencil have been extended.

The mapping of skewsymmetric matrices to either skewsymmetric or symmetric ones has received some study. Conditions, related to the Lyapunov mapping, that a symmetric matrix be the image of a skewsymmetric one have been found. Information on the invariant factor structure of a general matrix can be obtained from the skew \rightarrow skew mapping; this "linearizes" and offers interesting computational possibilities for solution of this difficult problem which is known to be computationally unstable.

A basic component of the work has led to a new formulation and solution of a very old problem in matrix algebra: finding the commutant of two matrices. In doing this, the classical similarity structure theorem for a matrix was formulated entirely in terms of a space having as dimension the degree of the minimum equation of the linear operator.

The goal of this specific project, regarded as part of general research in computational or algorithmic algebra, is to create a coherent and effective theory and exposition of the algebraic relations underlying the Lyapunov criterion, unifying and extending it as necessary, to make the results readily

usable in control theory for use by designers. Further, the literature and problems of stability analysis are to be effectively brought to the attention and interest of competent mathematicians and computer scientists.

3.3.3 Numerical Methods in Functional Analysis

The general problem of taking advantage of the theory of complex variables to construct methods for numerical problems involving real analytic functions is being studied. Although arithmetic calculations with complex numbers are generally more time-consuming than those with real numbers, the use of complex variable theory can often effect a net computing economy or a more stable algorithm. In a large number of problems handled by our computer the functions involved are analytic. These can often be evaluated in the complex plane and there is no *a priori* reason for avoiding this.

Recent work has concerned the application of Hilbert transform theory to numerical quadrature and numerical closed-contour integration. Techniques for numerical quadrature, stable numerical differentiation, calculation of Fourier transforms, and location of zeros have been developed. Two algorithms for evaluation of a set of normalized Taylor coefficients of an analytic function have been developed.

3.3.4 Solution of Nonlinear Equations

Refinements of mathematical models of the physical world frequently replace linear equations and systems of equations by nonlinear ones. It is thus important to have available an arsenal of numerical techniques to solve such equations. These equations are invariably hard to solve, usually because it is necessary to employ time-consuming iterative procedures to improve earlier estimates of the solution. Furthermore, as in parameter studies, solutions may be required for many nonlinear equations. These equations appear in a number of contexts, often as auxiliary parts of broader problems.

Several efficient new methods for finding roots of a single nonlinear equation have been discovered. Two of these procedures achieve fourth-order convergence with one derivative and two function evaluations per iteration step. Similarities among these two methods and a previously known third method due to Ostrowski led to the finding of an entire family of such efficient fourth-order methods. Furthermore, in each case, the derivative is to be computed at a point where the function value has just been found; this may simplify the calculation.

A variety of new methods utilizing alternate computed values of the given function and its derivative have also been found. These are comparable to the well known secant and Muller interpolation methods. They may be superior, however, when the derivative is readily computable.

One of the most common schemes for solving a nonlinear equation is the Newton-Raphson method. Over two steps it enjoys a fourth-order rate of convergence. A newly derived procedure that adds a correction term every other step turns out to be of fifth order with essentially no additional work.

3.3.5 Numerical Differentiation

An investigation has been carried out on the use of numerical differentiation in computational algorithms. Historically, numerical differentiation has a very bad reputation. This is because of the phenomenon of amplification of rounding error in the differencing process. Recently it has been shown that, when complex function evaluations are allowed, a simple, numerically stable process for numerical differentiation may be constructed. Two automatic routines that require complex function values, ENTCAF and ENTCRE, have been published in the algorithms section of the Communications of the ACM; a numerical differentiation routine based on real function values is under construction.

The algorithms ENTCAF and ENTCRE (Evaluation of sets of Normalized Taylor Coefficients) are essentially numerical differentiation routines using complex function values. In cooperation with G. Sande (The University of Chicago) these have been rewritten to incorporate data manipulation using a fast Fourier transform technique. The ACM is making these algorithms available on magnetic tape.

The MIPS method for Fourier coefficients has been extended. This is a method for calculating sets of Fourier coefficients when approximations to the derivatives of a related function at the end points are known. The technique was previously available only for "well behaved" functions over an interval coinciding with the basic period of the periodic function. The extensions involve an arbitrary interval, functions having algebraic singularities, and functions having sudden high peaks due to nearby poles in the complex plane. The nature of the singularities and poles must be known.

The MIPS method requires derivatives, which are readily provided by ENTCRE. However, it could be equally well used with only rough derivative approximations. So, in cases in which complex function values are not available, an automatic numerical differentiation routine based on real function values would be useful. While the class of problems in which it may be useful is more limited (because it is very much less accurate than ENTCRE), the class of functions which it can handle is larger, as it includes those for which complex function subprograms are not readily available.

3.3.6 A System for Computing Matrix Eigenvalues and Eigenvectors

Three central problems in computational linear algebra are the solution of the matrix equations

$$\begin{aligned}AX &= X\Lambda \\AX &= BX\Lambda \\AX &= C\end{aligned}$$

The first two equations represent the standard and generalized eigensystem problems, respectively, and the last represents the solution of a system of linear equations.

The programs for numerical solution of the standard eigensystem problem, collectively called EISPACK, are Fortran codes derived at Argonne from

Algol originals published in "Handbook for Automatic Computation, Volume II, Linear Algebra," by J. H. Wilkinson, C. Reinsch (Springer-Verlag, New York, Heidelberg, Berlin 1971).

AMD is pursuing a multi-faceted effort to enhance the usefulness of the EISPACK codes. This effort has resulted in five principles which have guided the development of EISPACK as a portable systematized collection of codes.

i) The codes should be available in a widely used, relatively machine-independent source language.

ii) Codes solving similar problems should have similar calling sequences and should be stylistically similar.

iii) The codes should be thoroughly tested in varied environments, preferably by means of programs developed to evaluate their performance.

iv) Where a sequence of several codes is required to solve a problem, or where selection of codes well-suited to solve a problem is complicated, supervisory programs should be developed which act as interfaces between the user and the codes by automating the sequencing or selecting.

v) The codes should be well documented.

The development of EISPACK has consisted, and will consist, of applying these principles to the following goals:

a) to produce a systematized collection of programs (including a control program EISPAC to simplify their use) for the standard eigenproblem $AX = \lambda X$;

b) to extend the above collection to include codes for the generalized eigenproblem $AX = B\lambda X$ and codes specialized for band matrices; and

c) to investigate the problem of devising general techniques for adapting the programs in these packages to handle large matrices, i.e., those that are too large to be stored in the primary memory of a computer.

The systematization of the codes for the standard eigensystem problem (goal (a)), according to the five principles, has been completed, and EISPACK satisfies principles (i) and (ii). The testing in principle (iii) is continuing in conjunction with the field test sites of the NATS project (see sec. 3.3.8).

Performance evaluating programs (themselves somewhat systematized) were prepared; also, from the recommendations developed in the NATS field testing program, a second edition of the EISPACK codes was completed and released for testing.

Corresponding to principle (iv), a modular control program, called EISPAC without a "K", has been developed. EISPAC allows the to substitute,

for the five or six calls to the EISPACK routines, a single call to EISPAC with parameters describing, in terms familiar to the user, the problem he wishes to solve. In this way EISPAC frees the user to concentrate on the details of his problem rather than on the details of the eigensystem programs.

The documentation of EISPACK (principle (v)) currently consists of detailed documents for the codes and EISPAC. A User's Guide is being produced.

3.3.7 Numerical Subroutine Library

Algebraic language compilers created by systems programmers act as an interface between computers and users, making the computer respond to commands based upon simple mathematical or statistical terminology. The creation of numerical subroutine libraries carries the interface one step further by making available in the algebraic language many of the non-trivial operations, symbols, and functions commonly used in mathematics and the physical sciences. Because such libraries are widely used in solving practical and research problems, it is important that library routines perform the expected computations both efficiently and accurately. Three goals of subroutine library development are

- development of techniques for the numerical evaluation of special functions,
- development of numerical techniques for data fitting and smoothing, and
- development of techniques for performance evaluation of mathematical software.

New minimax approximations have been developed for the Riemann zeta function and have been exploited in a subroutine that is many times faster and much more accurate than previous ones. A new technique for functions of two variables has been developed and used in subroutines for the irregular Coulomb wave function. The Coulomb routine gives results accurate to about 15 decimal places, in comparison to the previously available 4- to 5-place accuracy.

The Fortran library distributed by IBM for the System/360 computers was tested and results were made available (ANL-7666). Several replacement routines were provided for our users when these tests detected weak members.

A technique consisting of a family of methods depending on the minimization of certain functionals has been found for smoothing empirical data. Instead of assuming that the data conform to a certain analytic form (either locally or globally), as most smoothing techniques do, this one only assumes that the data correspond to a function which is smooth in some sense. The technique was designed for smoothing one-dimensional data, but can be extended to the two-dimensional case.

Also, new minimax approximations have been developed for the psi, or digamma, function, and the previously developed technique for the calculation of functions of two variables has been successfully applied to the incomplete

gamma function. Additional subroutines have been provided for the associated Legendre functions, certain vector addition coefficients, and the complex exponential integral.

Additional work on subroutines included the evaluation and preparation for local use of a number of subroutines developed at other installations. Routines for arbitrary precision floating point arithmetic (Stanford and The University of Chicago), inverse Gaussian and inverse error functions (The University of Chicago), the complex gamma function (The University of Chicago), and a normal random number generator (The University of Chicago) were involved in this effort. The Jenkins-Traub polynomial root-finder was also added to the library.

A study, with H. Kuki of The University of Chicago, of the implications of various schemes for founding, normalization and use of guard characters in computer arithmetic has been completed.

A general-purpose least squares fitting program obtained from the National Bureau of Standards has been modified for our library and then thoroughly checked. An alternate driver was also provided to handle certain commonly occurring least squares problems more efficiently.

As a preliminary step for the NATS project (see below), and in anticipation of their use at other AEC installations without IBM equipment, elements of our library of special function subroutines are currently being revised and versions are being prepared for use on CDC 6000 series and UNIVAC 1108 computers.

3.3.8 Collaborative Research Toward the Development of a Certified Subroutine Library

This project is funded by the National Science Foundation, NSF grant AG246. The following is the project summary as recorded by the Smithsonian Institution Science Information Exchange:

The Argonne National Laboratory, the University of Texas at Austin, and Stanford University will conduct a pilot project to explore means by which scientific users of computers can collaboratively test and certify mathematical software and make results available to the computing community. The project involves (1) intensive testing and refinement of a selected set of basic mathematical routines with field testing by a larger group, and (2) the design, implementation and operation of a prototype distribution center.

This is a prototype venture whose purpose is to develop ways of supplying the scientific computing community with highly reliable subroutines. Selected software is tested first at the three principal institutions and then at field test sites. Routines of proven quality are certified and distributed from the Argonne Code Center. A collaborative testing methodology is emerging from the project.

Software selected for testing and distribution includes a collection of routines for calculating certain special functions of mathematical physics and EISPACK, a Fortran package of eigensystem routines based on Algol originals of Wilkinson, Reinsch, and their colleagues (see Sec. 3.3.6).

The report of the first year's activities in this two-year project was transmitted to the Office of Computing Activities of the NSF via the Chicago Operations office of the AEC on January 14, 1972. Reference may be made to that report for detailed information on the progress of the project.

3.4 Programming Languages and Systems

3.4.1 Automated Theorem Proving

Automated theorem proving is concerned with obtaining proofs of theorems from various fields of mathematics with the aid of a computer. The procedures we employ are refutation procedures, that is, the purported theorem is assumed false, and "proof" by contradiction is then sought.

A paper which proves theorems about maximal models and refutation completeness of an inference system based on the paramodulation inference rule appears in a volume in the series, "Studies in Logic and the Foundations of Mathematics," published by North-Holland. Paramodulation is a rule which can be viewed as a generalization of equality substitution.

A theorem-proving program RW1 employing the inference rules paramodulation and/or resolution has been completed. Paramodulation has been known to provide the user with "built-in" equality and to allow him to omit various axioms which ordinarily must be included to characterize the equality relation. Proofs employing paramodulation are generally shorter and more natural than those employing resolution.

A system has been completed, based on RW1, which allows the user to enter and receive various types of information from a remote terminal. Although the system is mainly for the purpose of obtaining proofs of various mathematical theorems, in addition to the information describing the theorem under consideration and various conditions under which proof is to be sought, information about program changes and I/O options can be included.

A number of experiments are being conducted to determine the effects of various combinations of strategies and inference rules upon proof search efficiency. Various additional strategies and options are being designed and implemented for RW1. Some examples of options and/or strategies are the option to suppress paramodulation from and/or into a variable, the restriction strategy of demanding that the proof be an input proof, and the use of demodulation if and only if the user so commands.

3.4.2 Extensible Languages and Language Definition Methods

An extensible programming language is one that contains significant facilities which enable a programmer, working within the language, to define new language elements. The value of this is that the code defining the new

language element need be given only once, while it may be referenced many times. The amount of time spent in detailed coding is reduced and the programmer is able to construct his program at a higher level, thus reducing the chance of error.

A method of language description suitable for describing the extendible language has been developed, along with a suitable treatment of identifier binding so that an identifier can be used in different blocks for different purposes without any conflicts or unexpected effects arising during macro expansion.

The method of language description treats a syntactic definition as a modification of the language's *concrete syntax*. The concrete syntax describes the correspondence between the ordinary source text of a program and a tree-structured form of the program called the *abstract source program*. It is a formal analog of the syntactic-analysis part of a compiler. The method also treats macro procedures as rules to be applied during *translation* of the abstract source program into an *abstract object program*.

The complete attribute structure of the language is part of the syntax, being mostly described by special predicates and function definitions which we call *attribute rules*. The relevance of these attribute rules to language extension is that they indicate precisely what information is available during translation, and hence during macro expansion.

After much trial and error a method of identifier binding has been found which seems satisfactory in all respects. Formally, the semantics of identifier binding are most easily described by a combination of a copy rule (generate new identifiers and substitute them in a block being translated) and an environment which records the declared meaning of each identifier. However, we also have a semantically equivalent algorithm which computationally is much faster. Some theorems have been proved which indicate the reliability of the binding method.

4.0 COLLABORATIVE RESEARCH AND DEVELOPMENT

The computer has proven to be an invaluable tool in support of research. The Applied Mathematics Division conducts computer science research and applies known techniques of computer science to problem solving. Programming systems have been developed to assist the research and development activities of the Laboratory, and they have enabled the solution of many difficult and important problems. Some of the efforts in which computer science (computer programs or programming systems) has played an important part in solving engineering and scientific problems are described below.

4.1 Argonne Braille Machine*

A joint project by the Engineering and Technology and the Applied Mathematics Divisions is the development of a device which may make obsolete the bulky and costly Braille book and substitute for it a small reel of magnetic tape. A conventional Braille book, embossed on heavy paper, is about fifty times as bulky as its inkprint counterpart. In contrast, a large book encoded on magnetic tape will require only as much space as a typewriter ribbon.

The Braille machine takes symbols recorded on ordinary magnetic tape and converts them into patterns of upraised Braille dots on a plastic belt that the device moves past the fingertips of a sightless person. The reader can adjust the speed of the plastic belt at will. After the symbols move beyond the reader's fingers, the device "erases" the dot patterns by depressing them and raises new dots for the next loop. The belt is made of a special durable plastic that can be used for months before replacement is necessary.

With the Braille machine and a plug-in keyboard, a user can also "write" his own letters, notes, etc., on magnetic tape; these can be "played back" on his own or on a correspondent's machine.

For the blind reader, the Argonne Braille Machine offers hope of a vast increase in the amount of literature available to him, and also the promise that reading will be less difficult. Through these innovations, the cost of reading material for sightless people can be cut to a small fraction of what it is now; a far greater volume and variety of literature can be made available.

Prototype engineering models and a field test model of the Braille machine have been constructed and tested; thirty machines will be built for field test purposes in order to determine the final machine configuration.

4.2 Great Lakes Studies

Several fluid-dynamical problems associated with Lake Michigan and the other Great Lakes are being studied. The goal of the studies is to gain a better understanding of the dynamics of the lakes in order to assess the effects of man's activities on the lakes.

* Supported by HEW

a) Lake Circulation

This project concerns the theoretical study of the hydrodynamical and thermodynamical processes in the Great Lakes. The fundamental problem is to gain sufficient understanding of the lakes in order to develop practical techniques for predicting the large scale currents, wind set up effects, and pollutant dispersion patterns in the Great Lakes. The research activities are devoted to the systematic development of models of the Great Lakes with particular emphasis upon understanding the reliability and limitations of each successively more complex model. Work is being performed in the following areas.

i) State-of-knowledge survey. Because of the complexity of the dynamics of the lakes and the meager amount of available data, information from many sources is being gathered and analyzed in order to construct and evaluate numerical models.

ii) Bathymetric data file. A data file of the bottom configuration and shoreline of Lake Michigan is being constructed from navigation charts and other sources.

iii) Steady-state studies. As a first step in the development of theoretical models of Lake Michigan, a steady-state uniform density numerical model with realistic basin is being developed. A two-dimensional formulation of the problem in which the horizontal mass transport and the surface deflections are the major dependent variables is being used. The motions in the system are driven by wind stress using both idealized wind fields and some examples from weather charts.

iv) Time-dependent motions. A study of time-dependent motions formulated similar to the above steady-state study will be conducted. The effect of simple time-dependent wind fields and lake oscillations (seiches) will be studied, and the storm problem will be considered in more detail than in previous work.

b) Thermal Plume Studies

The effects of a discharge of heated lake water from a lakeshore power plant are largely unknown. ANL is active in the study of the physical, biological, and meteorological aspects of thermal plumes at existing lakeshore power plants. Work in AMD is concerned with the organization, analysis, and display of temperature and current data.

Temperature measurements are made from a boat which travels through the plume several times, giving a number of transects.

Unfortunately, to obtain enough transects to give an unambiguous picture of the plume using only one or two boats takes so long that major changes in the plume occur during the process of measurement. Thus, a purely experimental program either requires more boats and personnel than are presently available, or it does not provide adequate data.

In principle, given the bottom topography of the lake, ambient currents and temperatures, the flow through, and temperature at the outfall, one

could use the Navier-Stokes equations to calculate the isotherms. Past experience has shown that in practice this approach is not feasible.

Present work in the Applied Mathematics Division is concerned with development of some less expensive compromise between the two costly extremes of extensive measurement and ab initio calculation.

Variable Mesh Techniques

Many fluid dynamical problems have important 'boundary layer' regions in the domain of interest. These regions of rapid change in the solution must be adequately resolved in order to compute the correct overall solution. In performing an efficient numerical calculation, a smoothly varying mesh size is often required. The means of generating an appropriate mesh will usually vary with the problem. The research method employed is a combination of experimental calculations on specific applications to discover difficulties and theoretical analysis of numerical methods.

Work has been completed in which an automatically determined variable mesh was used to study a problem in linear hydrodynamic stability theory. Mathematically, the problem is a two-point ordinary-differential eigenvalue problem that is computed by solving the matrix eigenvalue problem approximating the differential equation. A 'boundary layer' zone occurs near one of the boundaries and a suitable variable mesh is selected automatically by restricting the absolute change in the solution between successive mesh points to below a predetermined value. The method has been applied to the problem of the stability of plane Poiseuille flow, and several uncertainties occurring at large Reynolds numbers have been resolved.

4.3 Library Acquisition System

The library acquisition system, prepared in cooperation with Argonne library personnel, provides facilities for file management, for order placement, and for general library record keeping. The system permits the entry of bibliographic information, the initiation of purchase orders, and review of the status of books that have been ordered.

Bibliographic information is entered into the system upon the recommendations of Argonne branch librarians and other members of the staff. Once sufficient information has been entered in the file, the bibliographic entry for this book will be printed on a selection list when the list is requested by the library.

Requests may be initiated either by the library or by individuals. The request entry must specify the book, the requestor's name and address, the applicable cost code, the publisher, and the number of copies. The request may also specify a vendor, but if not, the vendor listed in the bibliographic entry will be used. Each separate order appears on an individual request card. When the program is run through its ordering cycle, a purchase order will be generated for each request.

In addition to the bibliographic file, the master tape contains a vendor file. Each vendor entry contains a code, a name and mailing address,

a number of Argonne's purchase order, the amount of any discount allowed by the vendor, and an expedite interval. The expedite interval is determined by the acquisitions librarian based on the turnaround time of the individual vendor. On each update cycle, the program will, upon request, flag any orders that have been outstanding for longer than their expedite intervals and prepare expedite letters.

The system provides extensive diagnostics to indicate incomplete or improper information. Besides accepting bibliographic, vendor, and request information, the system will accept entries that indicate the receipt and cataloging of each book. The system is therefore able to monitor the history of any book from initial recommendation and ordering to final accounting and cataloging.

After the final disposition of all outstanding requests for a book, the entire entry is passed to a historical tape. The system allows use of a RESCUE time-sharing terminal (see Section 5.5) to build program input in the form of card image files. This input can be submitted directly into the batch system when the program is run.

A special user's manual for library personnel and a topical report on the overall system have been written.

4.4 The Argonne Reactor Computation (ARC) System

A reactor computation generally involves a series of large, long-running programs executed in a logical order. Each program in the series requires a portion of its input data to be produced by programs executed earlier in the series. A physicist performing a calculation must make logical decisions, based on the output at any given point in the series, concerning what kind of calculation to do next. Thus, the concept of a modular system in which the physicist can "pre-program" his decisions arises.

A useful concept for reactor calculations is a system in which the modules are large collections of subroutines, that is, programs or overlays, that can reside on direct access storage devices. The Argonne Reactor Computation (ARC) System, developed by the Applied Mathematics Division for the Applied Physics Division, is such a modular system. It consists of a library of computational modules with specified input and output interfaces. Reactor calculations are directed by means of a Fortran program, called a path, that executes programs and makes decisions concerning the course of the calculation. A path, therefore, functions as a monitor directing a computation through a collection of modules. Intra-module communication is through named collections of data that have been described in a glossary that lists the dataset name, its contents, and its format.

4.4.1 Development

The original specifications for the ARC System included the following:

- All programming to be done in FORTRAN IV
- Machine independence

- System extendability
- Use of standard FORTRAN I/O.

The first approximation, begun in 1965, was a large overlay program together with a data glossary defining the input and output data structure for each module in the system. This version was as close to being machine-independent as possible. It was economical, since no functions appeared twice. Programmers were able to work on their computational modules and physicists could design segments to direct these computations.

This overlay approach was discarded for several reasons.

- While it was possible for programmers to work in this manner, it was inefficient, since everyone's programming errors affected everyone else.
- Duplicate names were not allowed for subroutines, and thus programmers had to communicate every new subroutine name to everyone else.
- When any change was made, the entire system had to be reconstructed.
- Modules could not call other modules that appeared on the same level.

The next version to be developed allowed the ARC System to run on an IBM/360 model 50-75 using PCP (Primary Control Program) or MFT (Multiprogramming with a Fixed number of Tasks). A small amount of assembly language coding transformed the overlay "system" into a system in which each computational module became an executable program in a library. Very little recoding was necessary within the computational modules and some power was gained; any module in the system could now invoke any other module. Thus, any complete computation could become a subcomputation of any other. Two subroutines, LINK and LOAD, were developed to remove the deficiencies listed for the overlay version.

The third version of the ARC System provided the capability of running under MVT (Multiprogramming with a Variable number of Tasks). A resident I/O module was developed to save space and to eliminate core fragmentation. The I/O module involves a subroutine that traps all of the I/O calls generated by the compiler. This routine also LOADs the I/O module if it is not in core and locates it if it is, using little time. The I/O module is invisible to the user, who simply writes Fortran I/O statements.

4.4.2 Structure

The ARC System contains three types of modules: computational, control, and system,

The computational modules are calculational units that are directed by the control modules and supported by the system modules.

The control modules (paths) are written in Fortran, and therefore all of the power of the compiler is available for directing the computations. As a consequence, computational modules can be executed repetitively, and the course of a complete reactor computation can be determined by intermediate results.

The control modules also have system responsibilities. They must call routines to LOAD the system routines, initialize system tables, and protect the initialization throughout the run.

The system modules are required to interface with OS/360 and to build and maintain tables. They are of two types:

- Resident system modules, which build and maintain tables required by the ARC System.
- Transient system modules, which process input data into datasets for use by computational modules.

4.4.3 Libraries

A flexible library system was provided to handle the large amounts of code available and to facilitate the production and maintenance of modules. The library system provides for the updating of source code, the building of submodules from groups of subroutines, and the construction of complete computational modules from these submodules. Four libraries were constructed on direct access storage to do the following:

- Store all source statements in related members of 500 cards or less.
- Store the compiled versions of the source components.
- Store the instructions that direct the construction of the modules from the compiled components.
- Store the executable load modules.

4.4.4 Cataloged Procedures

Cataloged procedures for library maintenance were developed. Changes in a given member of the source statement library, in the compiled version of that member, and in executable modules using the member can be made using simple control cards.

Cataloged procedures were also written for all paths. The cataloged procedures incorporate the standard DD cards for each path, so that the user need specify only a few procedure control cards in addition to his card input.

4.4.5 Computational Capabilities

The ARC System is open-ended; new computational modules can be added as they are developed. At the end of Applied Mathematics Division's involvement, the system included nine "standard" paths to perform common calculations.

These included multigroup cross section preparation paths, one- and two-dimensional diffusion theory paths, one- and two-dimensional diffusion perturbation paths, one- and two-dimensional transport theory paths, and a burnup and fuel management path. Each of these paths invokes the computational modules in an order that is frequently used; the user of each path has run-time options concerning which modules he wants to use. Users also can write their own paths using the computational modules available.

The computational modules perform input, computation, edit, and adjunct functions. Among the modules developed by AMD are a neutronics input processor, two cross-section homogenization modules, one- and two-dimensional diffusion calculation and search modules, one- and two-dimensional transport calculation modules, one- and two-dimensional diffusion perturbation modules, one- and two-dimensional neutron inventory modules, a fuel cycle analysis module, and early versions of the six cross-section generation modules.

The ARC System can be readily transported to those AEC contractors with OS/360 and is in use at the NRTS in Idaho on an IBM 360/75 and at the IBM Scientific Center in Palo Alto, California, on a 360/50. The ARC System has also been tested without changes on IBM models 85 and 195. A project called EXODUS, to study the transportability of the ARC System to CDC 6000-series hardware, has been completed (see below).

Capabilities of the ARC System and detailed descriptions of its modules and paths were documented in ANL reports ANL-7332 and ANL-7711 through ANL-7722. Further development of the ARC System is being carried on by the Applied Physics Division.

4.5 The Conversion of the Argonne Reactor Computation (ARC) System to CDC 6000-Series Computers (Project EXODUS)

The Argonne Reactor Computation (ARC) System, described above, was designed for and implemented on Argonne's IBM System/360 computer with the MVT (multiprogramming with a variable number of tasks) Operating System. Since many AEC and AEC-contractor installations use CDC 6000-series computing equipment, it was felt that the availability of a CDC 6000 version of the ARC System would make possible more widespread use of this system. An effort was launched, with the assistance of Control Data Corporation, with the following objectives in mind:

- a) to examine the practicability of producing a version of the ARC System operable on CDC machinery;
- b) to define the system requirements, both hardware and software, for the 6000 series to support the ARC System; and
- c) to implement and execute a portion of the ARC System on 6000 series hardware.

An extensive study of the ARC System's dependencies on the System/360 as well as the capability of the 6000 series to support the ARC System was made. A key achievement was the establishment of an efficient operating environment for the ARC System by accommodating the differences between

the IBM and CDC operating systems. This involved redesign of the modules forming the system aspect of the ARC System. Some 25,000 cards of computational source code were also converted from IBM 360 Level H Fortran to the CDC Fortran Extended (FTN) language. This portion of source code represented all the modules necessary for a two-dimensional diffusion theory computation. Because of the ARC System modularity, the conversion provided about one-fifth of the total ARC System capability in the CDC version.

The CDC ARC System implementation avoids features that are peculiar to local installations of the 6000 series operating system. Thus, there are no requirements for a particular CPU, or for particular quantities, sizes, or speeds of mass storage devices. The only restriction is that the CDC ARC System is designed for the SCOPE 3.2 monitor and makes use of properties of that operating system which may not exist in earlier ones.

4.6 Chicago Air Pollution Study

The Applied Mathematics Division provided support in the data-handling and computational phases of the Chicago Air Pollution study. This support concentrated on processing the historical data from which the study proceeded and on programming several prediction techniques.

Air quality data available consisted of SO_2 measurements made at fifteen-minute intervals at telemetry stations throughout Chicago since January 1966. Relevant meteorological data consisted of U.S. Weather Bureau measurements for the Chicago area and measurements made at Argonne at one-hour intervals over the same period. Actual SO_2 emission data for industrial sources was also included. A general information and computation system was developed, in the form of a collection of processing programs, to accomplish

- organization and preparation of the data file;
- data search and retrieval;
- development of computational techniques upon the retrieved data; and
- display of retrieved data, including some specialized graphical displays.

The system was designed with a flexible framework to permit both new data and new computational programs to be added easily. Some of the computational programs that have been developed are

- a statistical prediction technique that uses multiple discriminant analysis,
- a statistical prediction technique that uses a linear regression model, and
- a tabulation prediction technique based on the display of a frequency distribution.

A computer code for a physical dispersion model has also been developed. This model requires the simulation of the emission by both industrial and residential pollution sources and the calculation of the subsequent dispersion of the pollutants. A linear programming model for the control of pollution incidents has been generated on the basis of the physical model. The model determines the allocation of alternate fuels to major pollution sources and the extent of load-shifting by utilities, so that the severity of an incident can be acceptably reduced at minimal cost.

4.7 Remote Control and Data Analysis

More demanding experimental requirements and the addition of hardware to the 70-inch scattering chamber of the Physics Division's Tandem Van de Graaff accelerator have necessitated revision to the program for chamber control and data analysis. The new equipment permits computer readout of the detector arm angles. This has made it possible to develop a program that positions the arms in such a manner that they strike neither each other nor the beam collimator. These safeguards formerly had to be provided manually. A control program has been written that uses the new positioning program to automatically position the remaining arms, given the position of the master arm and the nuclear reaction of interest.

4.8 Information Storage and Retrieval

Two similar management-type PL/I programs have been written to handle personnel data. One, prepared for another division, produces reports from personnel data kept in a specially formatted card file. The use of cards for the file eliminates setup procedures on the S/360 and allows convenient submission of the program through a RADS remote access station. The second program, for use by the Applied Mathematics Division, posts time charges of AMD employees against the funds from which the division draws money. Design specifications have also been drawn up for a Define, Update, and Query System (DUQS), which will provide retrieval and revision of personnel data files through RESCUE on-line remote terminals. Two document files are being created with the Document Processing System (DPS): one covers completed program reports of the Systems and Applications Section, and the other catalogs IBM publications for the S/360. Inquiries can be made into either file to retrieve document information.

4.9 Hybrid Computing

Hybrid computing techniques which proved effective in aerospace work are now being applied to a variety of research endeavors at the Laboratory. The addition of the Fortran-programmable IBM 1130 computer to the hybrid facility expanded the capacity of the system, allowing more complex problems to be attacked. A library of subroutines for inclusion in the system has been developed. This will make certain often-used functions available and ease the programming burden that was inherent in the earlier hybrid system.

The hybrid computer has proved to be a very useful tool for investigating mathematical models of feedback control systems and of reactor dynamics. In addition, it has been used to investigate problems in meteorology and bio-engineering and the appropriateness of hardware random number generators as opposed to the more commonly used software random number generators.

The following are examples of the types of problems which have been solved using the facility.

- A multi-region, multi-group, reactor kinetics calculation which is an extension of the earlier hybrid work done in 1967. Further investigation is being made of hybrid multiplex methods, including their use for three-dimensional models.
- A mathematical model representing the build-up of pressure pulses in the human aorta.
- A program for digitizing meteorological bivane data and computing relevant statistics which includes a print-plot of the distribution function.
- A program to drive a solid-state random number generator and collect the results into digitized words which are punched on cards in a format suitable for entry into the IBM System/360 computer.

4.10 A Simple Information Retrieval System Based on PL/I

An information retrieval system has been developed that can be used on any data file that can be described in the following manner: (1) the file is composed of an arbitrary number of records, (2) each record is identified by a single unique key, and (3) the records are of fixed length.

The information retrieval system is written entirely in PL/I. In fact, the system really consists of a series of partially-completed PL/I programs. The routines are completed when the user supplies PL/I statements defining his needs. This was predicated by the decision to let PL/I be the query and report-generating language. That is, instead of writing our own query language and report-writing language, we have allowed the user to write PL/I statements and have let the PL/I compiler implement those statements. For instance, in order to define his data base, the user must supply a PL/I structure declaration. If a file is to be queried, the user must supply a PL/I "IF" statement defining the records that are to be extracted from the file. When the user wants to print reports, a PL/I statement to print the reports must be supplied.

Since the system is based on PL/I, the user has the full power of PL/I at each stage that he interacts with the system.

4.11 Hyperfine Structure in Mesic X-Rays

The program solves the Dirac equation for a muon in the various energy states of atoms with spheroidal nuclei. The effect of vacuum polarization is included as a modification of the electrostatic potential in the Dirac equation. The resultant (atomic) wave functions are combined with the relevant nuclear wave functions to compute the intensities and energies of the various components of the x-ray lines.

4.12 Hyperfine Coupling Tensors from EPR Data II

Given estimates for the components of the symmetric hyperfine-coupling tensor A_{ij} , the symmetric effective-nuclear-Zeeman-splitting tensor b_{ij} (a total of twelve independent parameters), and given the nuclear Zeeman energy; the program computes the EPR hyperfine splittings for various orientations of the single crystal relative to the applied magnetic field. The sum, F , of the squares of deviations of the observed splittings from the corresponding computed values is then determined and a least-squares procedure used to adjust the components of A_{ij} and b_{ij} so as to minimize the value of F .

4.13 Temperature Distribution in a Cylindrical Fuel-Rod Assembly

The program computes the steady-state, radial temperature distribution in a cylindrical fuel-rod assembly of infinite length. It is assumed that the heat generation in the rod varies with radial position, and the thermal conductivity depends upon the temperature, porosity, and pore shape of the fuel material.

Temperature changes due to swelling of the fuel material are also computed.

4.14 Partial Differential Equations on a Curved Region

This program solves the time dependent partial differential equations involving temperature and fluid motion in a region with a curved boundary and curved hole. The equations are approximated by finite difference methods and the accuracy of the calculated function observed.

4.15 Studies of Plume Rise Data

Using 18 different approximations to observed plume rise data, this program calculates the standard deviations for the observed values and for all of the 18 sets of calculated values of plume rise. Correlation coefficients between the calculated and observed values are also obtained.

4.16 A Study of Arbitrary Regions and Their Effect on Solutions of Partial Differential Equations

The main purpose of this code is to provide a method of defining arbitrary planar configurations through input data and to supply relevant information at boundaries so that certain types of partial differential equations can be solved in the resulting regions.

4.17 LMFBR Plant Design Parameter Reporting System

The LMFBR Parameter Reporting System (LMFBRPRS) provides file maintenance, query, and report generation capabilities for a large file of data associated with plant design parameters.

The direct-access data file consists of report definitions and parameter titles, values, and references for a maximum of 9999 parameters for each of twenty plants whose designs are being studied.

Many options are provided for creating, modifying, and selectively printing data in flexible formats.

4.18 CEA Applications of the Generalized Information System (GIS)

A versatile file management system has been generated for the Center for Educational Affairs (CEA) using the IBM Generalized Information System. The two major data files created contain information on the people and the educational institutions that are participating in CEA programs. Information in the PEOPLE and SCHOOL files is related by using a unique code for each institution. Data descriptions are held in tables which are separate from the data and from the programs using the data. This technique and a high level procedural language enables the user to make simple or cross-file queries with a minimum knowledge of the programming concepts involved. A formal report capability is used to print lists of individuals and addresses suitable for standard printed output or for producing mailing labels.

5.0 COMPUTER CENTER

5.1 Acquisition of the Argonne National Laboratory IBM/360 Model 195 Computer System

The Applied Mathematics Division has acquired an IBM/360 model 195 computer system which is used by the staff of the Argonne National Laboratory.

This acquisition effort was begun in January of 1970 with a report from several task forces which investigated the feasibility of a joint Argonne National Laboratory and National Accelerator Laboratory computer center. In August of 1970, a formal "Report of the Study Group on an ANL-NAL Computer Facility" was prepared and released by the AEC. This report presented several alternative configurations, one of which was used as the basis for our system. In September of 1970, a questionnaire was prepared and submitted to all the users of the Argonne computers which interrogated the users about their use of our system and their projected needs for the next two or three years. The data from this questionnaire was analyzed and used as the basis for the request for proposals from the computer manufacturers.

In November of 1970, two sets of benchmark job streams were begun. One set consisted of the major production application programs which are run by various divisions at Argonne. The second job stream consisted of a sample workload which was run at Argonne during a period of one week. The benchmarks were completed and released to the bidders along with the request for proposals in June of 1971. This request contained specifications for the software and hardware configuration that was required by Argonne to meet our growing needs.

Three manufacturers submitted proposals for the new computing system: Control Data Corporation, International Business Machines Corporation, and Texas Instruments, Inc. In order to qualify for consideration, all manufacturers were required to run our benchmarks. The results of the IBM run showed that their model 195 computer was capable of running 6.2 times the workload of our 360 model 75 computer system. The applications programs ran between 6 and 12 times faster on a 195 than they did on the 75. In August of 1971, the results of the CDC run showed that the CYBER 76 was capable of doing 6.8 times the amount of work than an IBM 360 model 75 system could do. The applications programs ran between 7 and 12 times faster on the CYBER 76 than on the IBM 360/75. TI did not run the benchmark problems and subsequently withdrew their bid.

The proposals from the three manufacturers were returned in the middle of July in 1971. They were evaluated on a technical basis by the staff of the Applied Mathematics Division, and the results of this evaluation were made available to the Atomic Energy Commission which negotiated the contract directly. On June 9, 1972, the Atomic Energy Commission announced that the Argonne National Laboratory computer system would be an IBM 360/195.

The formal contract between IBM and the Atomic Energy Commission was signed. A large effort was mounted to remove the old Control Data Corporation 3600 computer system and to modify the computer room so that it could support the Model 195 system. This modification involved additional air conditioning

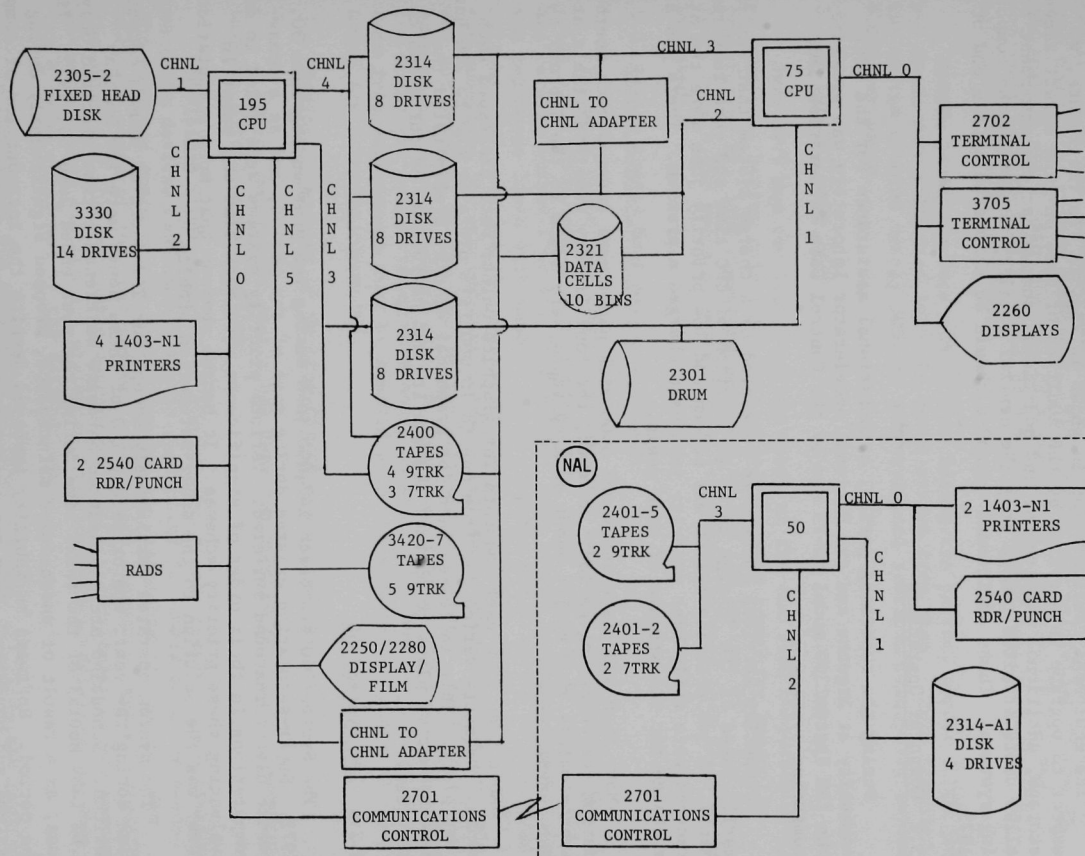


Figure 1. New System Configuration

equipment, additional electrical equipment, and relocating some of the remaining IBM computer equipment.

The equipment configuration is shown in Fig. 1. In the future, we expect to upgrade this system by the addition of more on-line direct access storage, additional tape units, and additional communications equipment to allow users at sites remote from the central facility to access the computing systems. These additional upgrades should be completed by the end of 1973.

5.2 Computer Operations

During the reporting period, computational assistance for the user community at Argonne and the National Accelerator Laboratory was provided by the IBM System/360 model 50-75 and by the Control Data Corporation 3600 computing systems.

Computing services costs were recovered by a charge system that was primarily based on the "charge unit" (a function of CPU time and core requirement). A job priority system was set-up and low priority jobs were run at a reduced rate while high priority jobs were charged a premium. There was also a charge for the storage of tape reels.

More than 5000 tape reels and 3000 disk packs were mounted each month during the reporting period. However, the tape library remained stable at approximately 7000 reels; about as many tapes were added to the library as were purged from it.

More than 1200 user requests for graphics output were processed each month. Requests varied for from one to 10,000 film plots or one to 200 hard copy plots. This increased need for graphical display precipitated the development of plans to upgrade the quality and usefulness of our graphics services.

5.2.1 IBM System/360

The System/360 processed 247,000 jobs during the year ending June 30, 1972. Super-saturation existed during most of the period, and as a consequence user turnaround suffered. Various priority systems were tried to do computations in their order of significance, and much time was spent in evaluating these priority schemes. It became obvious that more computational power was the solution to the super-saturation problem.

The system operated continuously except for 262 hours of unused computer time during the year; approximately 120 of these hours were for holiday periods. Scheduled and unscheduled hardware maintenance time required only 5.6% (489 hours) of the total time during the year ended June 30, 1972. Time loss, as a result of unscheduled maintenance, dropped significantly during the period. Software reliability improved despite the introduction of complex systems and hardware. Jobs run per productive hour increased in each year, from 24 per hour in 1970 to 33 per hour in 1972.

Remote Access Device Systems (RADS), a locally developed remote I/O system, became very popular and was heavily used. By the end of the period, almost 2/3 of the input to the system (14,000 jobs per month) originated from one of the remote terminals. This system was maintained by the AMD engineering staff with the help of a contractor. Frequently, it was necessary to direct RADS output to the main computer complex because of saturation at some terminals.

Remote terminals were widely used during the period; almost 5,000 jobs per month were submitted into the batch system from them. Users enrolled in the system totaled nearly 500 and user terminal sessions frequently exceeded 8,000 per month.

5.2.2 Control Data 3600

June 1972 was the last complete month of the CDC 3600 computing system at Argonne. During this reporting period the user community gradually transferred its 3600 computing workload to the IBM System/360. For the year, over 4,000 hours of machine time (representing more than 27,000 jobs) was used.

5.3 Remote Access Data Stations (RADS)

The main effort for remote system entry has been the RADS system. Utilizing small computers as remote terminals, users are able to submit jobs to and receive output from the System/360. Each remote terminal communicates via telephone lines with another small computer which serves as a message switcher for entering the System/360 queue. The bulk of the System/360 jobs are submitted through the twelve remote terminals throughout the Laboratory and the terminal at the National Accelerator Laboratory. These terminals have significantly reduced the job turnaround time by providing quicker system entry and by providing more entry points. Unfortunately, in each case data from experiments must be handled prior to submission, since no experiments are directly connected.

5.4 Region Management of On-Line Direct Access Devices

A region management system has been implemented for scarce resources--namely, direct access devices.

Divisions (Cost Centers) of the Laboratory may reserve space (regions) on these devices, and such space is guaranteed for their on-going needs. The reserved space may be restricted by the cost-center to one or more activity codes of the cost-center. The region management system identifies the owner and the chargeable account of all of the datasets on the devices. Datasets within regions are protected from inadvertent deletion and they can only be scratched by the dataset owner.

To supplement the management of these devices, utilities are provided which enable the cost-center (user) to:

- 1) determine the amount of space available in their protected region, and the accounts with datasets in the region, and

- 2) determine all of their datasets that are on any on-line devices, and the characteristics of those datasets.

Other utilities enable the computer center to monitor the available space on the on-line devices and aid in restoring devices on which the Volume Table of Contents have been destroyed. Individual dataset use is monitored to provide information for more efficient use of these direct access devices.

5.5 Conversational Computing (RESCUE)

Several new features have been added to RESCUE, Argonne's conversational computing system attached to the IBM System/360 model 50. These features have increased the utility of interactive computing throughout the Laboratory.

A "dial-up" feature was added to allow users to connect to RESCUE via the Laboratory's telephone system. Dial-up incorporated both an automatic disconnect and a restart function. The automatic disconnect frees a line that has been inactive for more than ten minutes. Restart protects the user against the consequences of accidental disconnection by allowing him to dial again and recover his active storage.

Since RESCUE is intended more for the working scientist than for the computer expert, a system to provide explanatory information was introduced. This system can be invoked at any time by typing the "HELP" command. Unlike most such assistance schemes, HELP provides a response that depends on what the user was doing when he requested HELP. HELP information can be obtained at three levels of progressively greater detail. The initial HELP message presents the user with a short list of alternate paths he may explore: he may obtain a general description, a list of commands, or an explanation of any command. The second level HELP response gives the general description or the list requested by the user. The third level provides the description of a command. The HELP system is transparent--its use does not affect the working storage.

The RXPL compiler, a modified version of the XPL compiler was implemented. RXPL provides the capability of writing interactive processors for RESCUE in a high level language (i.e., PL/I). Prior to RXPL, processors had to be written in assembly language. The programmer had to follow well defined but sometimes difficult to understand conventions, unless he had extensive knowledge of the internal organization of RESCUE. Several applications processors have been written using RXPL.

6.0 THE ARGONNE CODE CENTER

Since 1960 the Argonne Code Center has served as a computer program information center and library for computer programs developed under USAEC sponsorship. Liaison with AEC offices, AEC-contracting establishments, universities, and other government agencies is provided by individual staff members designated as Code Center representatives.

The Center's program is in three parts. The first, information services, includes the preparation and editing of the computer program abstracts, the answering of technical inquiries, the reproduction and dissemination of the program package materials, and the compilation of bibliographies of computer program literature. The second, computer activities, encompasses the review and assimilation of programs into the master library, maintenance and testing of the library collection, and the development of ACCESS, the Argonne Code Center Exchange and Storage System, designed to automate the Center's service functions. The third part consists of cooperative efforts and research on programs, such as documentation and programming standards undertaken with our European counterpart the OECD NEA Computer Programme Library and our professional "user group," the Mathematics and Computation Division of the American Nuclear Society, and the development of procedures to facilitate program portability and effective program interchange.

During the period covered by this report the Code Center received 331 program packages for inclusion in the library collection and an additional 85 NEA library packages for distribution in the United States and Canada. At the same time 4,173 requests for program package material were filled. Supplements 1 through 6 of ANL-7411, the Center's Compilation of Program Abstracts, were published describing new programs and additional machine versions or revisions and replacements of existing library programs. In addition, a directory containing the names and addresses of the Center representatives and describing the computing facilities and environment at the registered installations was compiled and published as ANL-7497.

A computer software system is being written to automate the Center's operation; the acronym ACCESS (Argonne Code Center Exchange and Storage System) was chosen to identify this system.

ACCESS is intended to provide for the storage, retrieval, modification, and display of Code Center information. This information exists in six interrelated but dissimilar data bases:

- requests to the Center for computer programs;
- a directory, or table of contents, of the Center's current library collection;
- descriptive abstracts of the library programs;
- library "program packages" including the distributable material for each program--such items as the source program, object program or load module, input data for a sample problem, auxiliary data bases and routines, and control and comment information;

- statistics maintained by the Center for activity reporting, record keeping and management information functions; and
- data relevant to registered institutions or recipients of Center programs, such as their hardware facilities, mailing information, library holdings, and selective dissemination of information (SDI) profiles.

ACCESS is being implemented on the Laboratory's IBM 360 computer system in the PL/I and Assembler languages. Data bases reside on IBM direct access storage devices.

All six data bases have been established. The table of contents file and the abstracts file have been used routinely in the preparation of the Center's Compilation of Program Abstracts report. A preliminary version of the installation data base was used to prepare the FY 1971 annual report. Initial entries have been posted in the request file, and 318 program packages have been entered into ACCESS' largest and most complex data base. The statistics data base is the most recently established. It was initiated with the first use of ACCESS in filling requests during FY72.

Phase 1 documentation describing the table of contents, abstracts, request, statistics, and installation data bases has been prepared. File maintenance and report-generating programs have been written in PL/I and Assembler for all ACCESS data bases and detailed specifications for their documentation have been drafted.

Work with the American Nuclear Society has been in two areas--standards and benchmark problems. In collaboration with the ANS-10 Standards subcommittee two standards were prepared, "A Code of Good Practices for the Documentation of Digital Computer Programs,"¹ which is currently undergoing revision, and "Recommended Programming Practices to Facilitate the Interchange of Digital Computer Programs."² The Center maintains a collection of benchmark problems prepared by an ANS Mathematics and Computation Division committee in 1968. Additions to this document are in preparation.

Since the establishment of the NEA Computer Programme Library in Ispra, Italy, the two centers have collaborated in the development of specialized computer program bibliographies and program library procedures; NEA staff regularly visit the Argonne Center to participate in program testing and validation.

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7.0 PUBLICATIONS AND PAPERS

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7.2 AMD Argonne Reports

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 Edited by B. J. Toppel. Applied Mathematics Division Contributors: D. Bingham, G. Duffy, G. Jensen, L. Just, A. Kennedy, G. Leaf, A. Rago, P. Walker, J. Zapatka, and J. Zeman
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 E. H. Bareiss (6/67)
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 V. Luco and G. K. Leaf;
 Section VI-14, *Error Analysis of Linked Difference Equations*
 N. F. Morehouse and J. C. Carter,
 in Reactor Physics Division Annual Report, July 1, 1967 to June 30, 1968, Section VI, Reactor Computation Methods and Theory.
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A. M. Brues, A. N. Stroud, J. W. Butler, and M. K. Butler in Biological and Medical Division Annual Report, 1968, pp. 31-32.
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- ANL-7793 *Instrumentation Systems to Protect LMFBR Core Integrity*
W. C. Lipinski, C. E. Cohn, D. R. MacFarlane, T. P. Mulcahey, D. Okrent, K. G. Proges, W. C. Redman, J. B. Van Erp, and R. H. Vonderohe (3/71)

- ANL-7808 *The Argonne Library Book Acquisition System*
C. Harrison and W. J. Snow (2/72)
- ANL-7812 *IBM 1403 Printer Modifications for Computerized Braille Output*
E. L. Kolsto (7/71)
- ANL-7818 *Creation of Hierarchic Text with a Computer Display*
W. J. Hansen (6/71)
- ANL-7847 *SYN2D, A Flux-Synthesis Program Based on a Discontinuous Trial-Function Formulation*
V. Luco, G. K. Leaf, and J. C. Stork (6/71)
- ANL-7855 *The Numerical Solution of the Orr-Sommerfeld Equation at Large Reynolds Number*
T. H. Hughes (9/71)
- ANL-7881 *A Simple Information Retrieval System Based on PL/I*
M. R. Kraimer and R. K. Clark (12/71)
- ANL-7898 *Multistep Elimination over Commutative Rings*
E. H. Bareiss and D. Mazukelli (4/72)
- ANL-7914 *Low-Order Gauss-Christoffel Quadrature*
I. K. Abu-Shumays (2/72)
- ANL-7925 *Applications of Finite Element Methods in Reactor Mathematics. Numerical Solution of the Neutron Diffusion Equation*
H. G. Kaper, G. K. Leaf, and A. J. Lindeman (2/72)
- ANL/ES-CC-003, *Section 5.0, Applied Programming*, A. Kennedy, J. Gregory, and J. Anderson. *Section 6.0, Abatement Strategy and Economics*, K. Croke, A. Kennedy, and D. Parsons, in *Chicago Air Pollution System Model Third Quarterly Progress Report*, October 1968.
- ANL/ES-CC-004, *Section 5.0, Applied Programming*, A. Kennedy and J. Anderson, in *Chicago Air Pollution System Model Fourth Quarterly Report*, March 1969.
- Machine Classification of Fingerprints*, C. B. Shelman, Argonne National Laboratory Reviews, April 1969.
- ANL/ES-CC-006, *APICS, a Computerized Air Pollution Data Management System*
C. Chamot, A. S. Kennedy, E. J. Croke, J. J. Roberts, H. Moses, and J. B. Anderson (2/70)
- ANL/ES-CC-007, *Chicago Air Pollution Systems Analysis Program: A Multiple-Source Urban Atmospheric Dispersion Model*
J. J. Roberts, E. J. Croke, A. S. Kennedy, J. E. Norco, and L. A. Conley (5/70)

ANL/ES-6 *Wind-Driven Currents in a Large Lake or Sea*
G. E. Birchfield (7/71)

ANL/ES-7 *Air Pollution-Land Use Planning Project. Phase I. Final Report: July 1971*
A. S. Kennedy, A. S. Cohen, E. J. Croke, K. G. Croke,
J. C. Stork, and A. P. Horter (11/71)

ANL/ES-10 *A Compilation of the Average Depths of Lake Michigan and Lake Ontario on a Two-Minute Grid*
T. H. Hughes, G. E. Birchfield, and M. T. Matthies (1/72)

7.3 AMD Technical Memoranda

These reports, although intended for internal distribution only, are available on request from the Applied Mathematics Division, D221, Argonne National Laboratory, Argonne, Illinois 60439.

Number

- 124 *A Proposal for an Automated Visual Fields System*
C. B. Shelman (10/68)
- 125 *The Argonne Hybrid Computer Users Manual*
N. K. Natarajan, L. Amiot, and F. Maletich (1/69)
- 138 *Electro-Optic Measuring Systems Using Coherent Light Sources*
F. Sato, R. Vonderohe, and R. Foster (6/68)
- 141 *Generating Functions for the Exact Solution of the Isotropic Transport Equation. I.*
I. K. Abu-Shumays and E. H. Bareiss (2/67)
- 150 *Computer Directed Direct View Storage Tube Display System*
J. Becker (8/69)
- 151 *A Preliminary Report on the Research of the Visual Fields Problem*
G. Goldbogen (8/69)
- 165 *A Non-automated Environment for the ARC System*
S. D. Sparck and L. C. Just (3/68)
- 167 *A Film-Plotting Subroutine Package (FSP) for for IBM 2280 Film Recorder*
D. Carson (6/68)
- 168 *Attached Support Processor Dynamic Status Recorder Data Analysis System*
A. R. Hirsch (6/68)
- 169 *Numerical Study of the Collapse of a Perturbation in an Infinite Ocean*
W. Roy Wessel (6/68)
- 170 *Liberator IX*
D. Hodges (7/68)
- 171 *Natural Classification*
D. A. Woodward (1/69)
- 172 *Integrated Macro Processing in Procedural Languages*
M. Donald MacLaren (7/68)
- 173 *Updating FORTRAN Source Codes Tape-to-Tape on the IBM System/360*
S. M. Prastein (9/68)

Number

- 174 *A Formulation of Rayleigh-Schrodinger Perturbation for Computation to Any Order, and a Discussion of Its Convergence and Applications*
J. R. Gabriel (1/69)
- 175 *Generating Functions in Transport Theory*
E. H. Bareiss and I. K. Abu-Shumays (2/69)
- 176 *A Magnetic Tape Braille Machine*
J. Haasl and W. Lidinsky (4/69)
- 177 *Execution of Production Programs on the IBM System 360 Computer*
Cynthia Chamot (4/69)
- 178 *Keysort Filing System for the Computer Engineering Section's Catalog File*
F. Sato (4/69)
- 179 *Buffer In/Out Facility for System/360 Fortran*
M. Matthies (5/69)
- 180 *The Argonne Braille Translator*
L. Leffler and S. M. Prastein (5/69)
- 181 *A PL/I-to-Fortran Interface Routine*
M. Matthies (5/69)
- 182 *PRETTIERPRINT for LISP 360*
W. J. Hansen (5/69)
- 183 *Introductory User's Guide to the IBM Mathematical Programming System*
J. Wenger (10/69)
- 184 *A Research Oriented Computer Associated Interactive Graphic Display*
W. Lidinsky (8/69)
- 186 *MVT Accounting Routine for Release 17 of OS/360*
D. Snider (10/69)
- 187 *The Role of Computers in Power Reactor Design*
E. H. Bareiss (9/69)
- 188 *RADS System Organization*
L. Amiot, H. George, and J. Haasl (4/70)
- 189 *BSAMIO - A FORTRAN Callable Subprogram that Interfaces with the OS/360 BSAM Macro Instructions*
L. Just (12/69)
- 190 *Graphic Editing of Structured Text*
W. J. Hansen (1/70)

Number

- 191 *Some Subroutines for Producing Captioned Contour Line Plots and Line Graphs on Film*
W. R. Wessel (2/70)
- 192 *Unrestricted Factor Analysis*
J. Gabriel and M. Gabriel (5/70)
- 193 *Representation of the Moments of the Sample Mean in Terms of Moments of the Underlying Distribution*
R. Buchal, D. Phillips, and B. Garbow (4/70)
- 194 *Operating Procedures for Accounting Card Validity Check*
J. Burnett (4/70)
- 195 *The Boundary Layer Formalism for Convergent Series Solutions of the Wave Equation, with Reference to the Diffracted Field in the Shadow Behind a Smooth Convex Cylinder Part III*
R. Buchal (4/70)
- 197 *RXPL Reference Manual*
K. Dritz (5/70)
- 198 *Initial Objectives of ON-site Empirical Modeling of Thermal Plumes: A Preliminary Evaluation of a River Site and a Lake-Site Thermal Plume*
I. K. Abu-Shumays (5/70)
- 199 *On Multiburst Techniques in Neutron Time of Flight Spectroscopy*
R. Buchal and D. Phillips (6/70)
- 200 *Factorial Series Representations as Check Solutions in the Development of Special Functions Computer Subroutines*
R. Buchal and G. Duffy (5/70)
- 201 *ALICE - A General Purpose Image Processor Preliminary Description*
R. Barr, J. Butler, J. Haasl, D. Hodges, B. Kroupa, C. Shelman, and R. Wehman (9/70)
- 202 *Some Preliminary Support Programs for the ALICE System*
D. Hodges (10/70)
- 203 *Console Guide for the DISCOM Interpretative System*
C. Smith (9/70)
- 204 *Digital Handwired Pincushion and Dynamic Focus Correction*
R. Barr and D. Jacobsohn
- 205 *Retrieving Source Decks for the IBM Fortran Scientific Subroutine Package*
J. Wenger (12/70)

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- 206 *SLOB5, A Program for the Solution of Sturm-Liouville Systems by Means of a Hermite Interpolation-type Ritz Method*
J. J. Kaganove and G. K. Leaf (2/71)
- 207 *RADS Remote Station Organization*
C. Harrison, F. Salter, R. Schwanke, T. Murphy, V. Tantillo, L. Amiot, and R. Barr
- 208 *Phenomenological Interpretations of Baer* - Semigroups*
J.C.T. Pool (11/70)
- 209 *One-Dimensional Transport Code for the One-Group Problems in Plane Geometry*
E. Bareiss and C. Chamot (9/70)
- 210 *Analytic Methods in Three Dimensional Transport Theory*
I. K. Abu-Shumays and E. H. Bareiss (2/71)
- 211 *Spherical Harmonics and Legendre Polynomials*
I. K. Abu-Shumays and E. H. Bareiss (2/71)
- 212 *Fortran and Assembler Level Programming of the ALICE Film Scanner under Monitor Control*
J. W. Butler
- 213 *The Argonne Benchmark Problem Collection*
M. K. Butler, A. R. Hirsch, S. Katilavas and M. R. Kraimer
- 214 *Applications of Finite Element Techniques in Reactor Mathematics First Series: The Numerical Solution of the Neutron Diffusion Equation. Part I: Statement of the Problem*
H. Kaper, A. Lindeman, and G. K. Leaf (3/71)
- 215 *An Algorithm for the Transformation of Lagrangian to Eulerian Coordinate Systems*
A. J. Lindeman (4/71)
- 216 *Parameter Generation for the Two-Dimensional Space-Time Kinetics Code FX2*
G. K. Leaf and A. J. Lindeman (4/71)
- 217 *A Synopsis of a Literature Survey on Iterative Methods Utilizing an Approximate Operator*
G. K. Leaf (3/71)
- 218 *Remarks on the Possible use of an ADI-B² Iterative Procedure for Solving the Static Three-Dimensional Diffusion Equation*
G. K. Leaf (3/71)

Number

- 219 *Applications of Finite Element Techniques in Reactor Mathematics - Second Series: The Numerical Solution of the Neutron Transport Equation - Part I: Statement of the Problem*
H. Kaper, G. Leaf, and A. Lindeman
- 222 *Computational Solutions of Matrix Problems over an Integral Domain*
E. H. Bareiss (12/70)
- 225 *Introductory User's Manual for "SYMAP" Contour Maps*
M. Matthies (3/71)
- 226 *Waukegan Station Plume*
I. K. Abu-Shumays (5/71)
- 227 *Operating Procedures for the System/360/50 Remote Access Data System*
J. A. Burnett
- 228 *Thermal Plume Data Acquisition, Documentation and Initial Analysis*
I. K. Abu-Shumays, D. L. Phillips, and S. M. Prastein
- 230 *A Comparison of Time Sharing Services Available with a View to the Next Computer Acquisition*
R. Krupp and C. Smith
- 232 *AL Monitor for the ALICE Film Scanning System*
J. W. Butler

7.4 Symposium Presentations and Papers Presented

1. *Software for the Elementary Functions*, by E. H. Bareiss, Mathematical Software Symposium (by invitation), Purdue University, April 3, 1970.
2. *Software for the Elementary Functions*, by E. H. Bareiss, Central Ohio Chapter ACM, Ohio University, Columbus, Ohio, April 13, 1970.
3. *Software for the Elementary Functions*, by E. H. Bareiss, Southwestern Michigan Chapter ACM, Western Michigan University, Kalamazoo, Michigan, April 14, 1970.
4. *Conference on Transport Operators in Three Space Dimensions*, by E. H. Bareiss, International Congress of Mathematicians, Nice, France, 1970.
5. *Conference on Linear Equations over an Integral Domain*, by E. H. Bareiss, International Congress of Mathematicians, Nice, France, 1970.
6. *Matrix Inversion over an Integral Domain*, by E. H. Bareiss, Institute Josef Stefan, Ljubljana, Yugoslavia, 1970.
7. *The Numerical Solution of the multigroup diffusion equation with the finite element method*, by H. Kaper, University of Illinois, Urbana, Illinois, 1972.
8. *Numerical Approaches to the Transport Equation and Computational Experimentation*, by E. H. Bareiss, Los Alamos Scientific Laboratory, Los Alamos, New Mexico, 1971.
9. *Computational Solution of Matrix Problems over an Integral Domain*, by E. H. Bareiss, Second Symposium on Symbolic and Algebraic Manipulation, Los Angeles, California, 1971.
10. *Numerical Solution of the Transport Equation*, by E. H. Bareiss, Symposium on Numerical Solution of Integral Equations, SIAM Fall Meeting, Madison, Wisconsin, 1971.
11. *Guidelines for Automatic Quadrature Routines*, by J. N. Lyness, IFIP Congress, Ljubljana, Yugoslavia, 1971.
12. *The Solution of Boundary Value Problems in Partial Differential Equations*, by J. N. Lyness, University of Liverpool, England, 1971.
13. *An On-Line Data-Acquisition Program for Nuclear-Physics Experiments on the Argonne Tandem*, by J. Tippie, Nuclear Science Symposium, San Francisco, California, 1971.
14. *The Neurotron Monitor System*, by R. A. Aschenbrenner, FJCC, Las Vegas, Nevada, 1971.
15. *MIRAGE, A Microprogrammable Interactive Raster Graphics Equipment*, by W. P. Lidinsky, IEEE Computer Conference, Boston, Massachusetts, 1971.

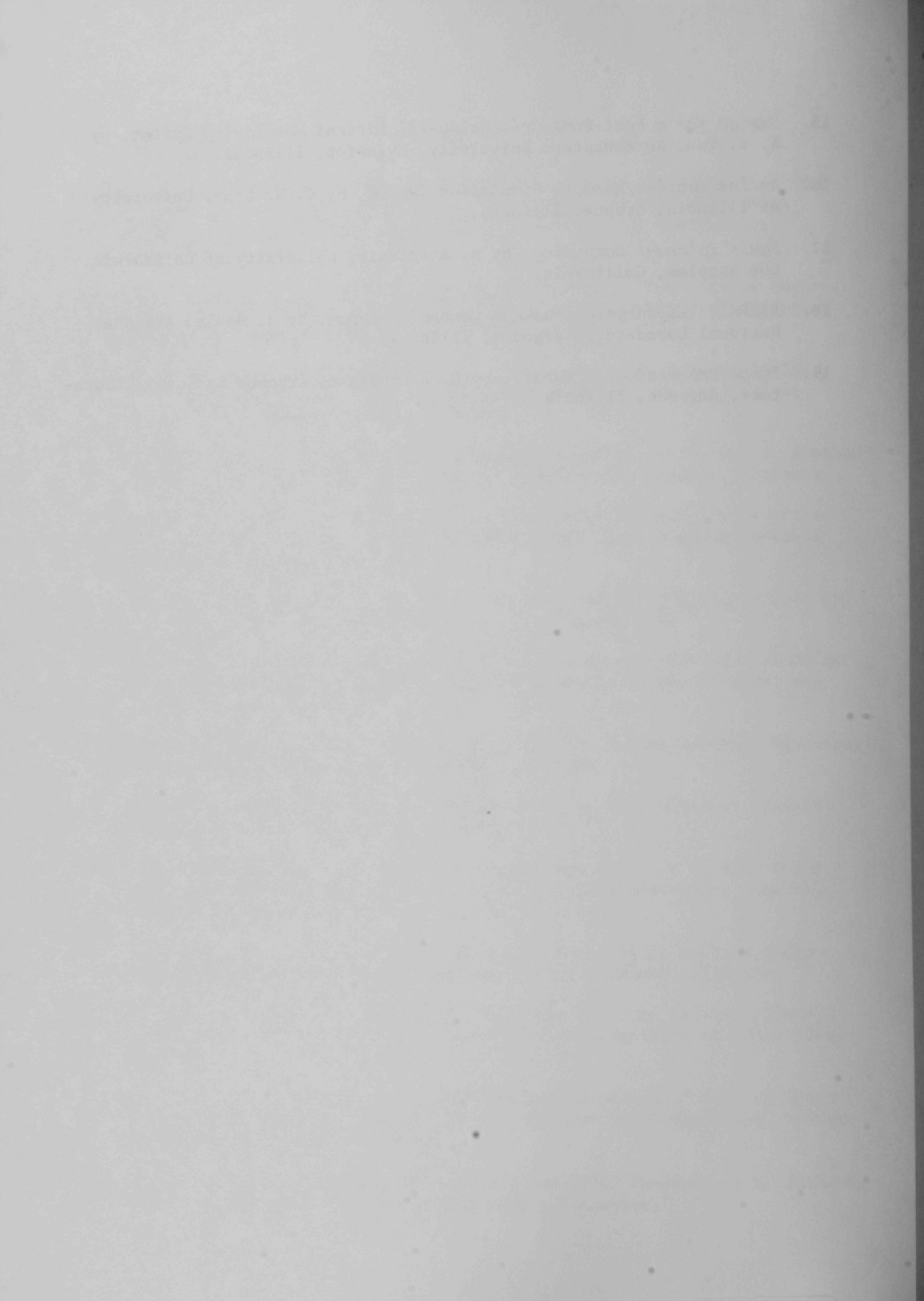
16. *Free and Forced Convection Processes at the Ocean-Air Interface*, by S. A. Piacsek, Stanford University, Palo Alto, California, 1971.
17. *Variational Methods for the Integral Transport Equation*, by I. K. Abu-Shumays, University of Illinois, Urbana, Illinois, 1971.
18. *Approximations for Computer Library Programs*, by W. J. Cody, Symposium on Approximation Theory, University of Toledo, Toledo, Ohio, 1971.
19. *Mathematical Models for Physical Random Number Generators*, by J. M. Cook, 130th Meeting of the Institute of Mathematical Statistics, May 5, 1971, Columbia, Missouri.
20. *Calculation of Fourier Coefficients Using Möbius Inversion of Poisson Summation Formula*, by J. N. Lyness, University of Toronto, Toronto, Canada, 1971. (Also presented at several other scientific and educational institutions in the U.S.)
21. *Has Numerical Differentiation a Future?*, by J. N. Lyness, SIAM Conference, Seattle, Washington, 1971. (Also at University of Leeds and U.K.A.E.R.E. Harwell in England.)
22. *Guidelines for Automatic Quadrature Routines*, IFIP Meeting, by J. N. Lyness, Ljubljana, Yugoslavia, 1971.
23. *Some Topics in One- and Multi-Dimensional Quadratures*, by J. J. Lyness, Liverpool, University, Liverpool, England.
24. *Numerical Algorithms Based on the Theory and Complex Variables*, by J. N. Lyness, University of Liverpool, Liverpool, England, 1971. (Also presented at the Universities of Newcastle, Bradford, and N.P.L. Teddington, England.)
25. *Image Processing at Argonne*, by C. B. Shelman, University of Chicago Medical School, Chicago, Illinois, 1971.
26. *A New Approach to Numerical Transport and Diffusion Problems*, by H. Kaper, University of Wisconsin, Madison, Wisconsin, 1971.
27. *Computer Design for Numerical Analysis*, by W. J. Cody, Northwestern University, Evanston, Illinois, 1972.
28. *Computational Techniques Based on the Larczos Representation*, by J. N. Lyness, University of Kent at Canterbury, England, 1972. (Also at Royal Irish Academy meeting in Dublin.)
29. *Numerical Solution of the Multigroup Diffusion Equation with the Finite Element Method*, by H. Kaper, Oak Ridge National Laboratory, Oak Ridge, Tenn., 1972.
30. *Elliptic Boundary Value Problems and the Finite Element Method*, by H. Kaper, Virginia Polytechnic Institute, Blacksburg, Virginia, 1972.

31. *Some Timing Comparisons for Low-Order Finite Difference and High-Order Finite Element Solution Methods for the Two-Dimensional Neutron Diffusions*, by H. Kaper, Naval Research Laboratory, Washington, D.C., 1972.
32. *Evaluation of Mathematical Software*, by W. J. Cody, Symposium on Computer Program Test Methods, University of North Carolina, Chapel Hill, North Carolina, 1972.
33. *Measuring the Motility of Living Cells*, by J. W. Butler, IEEE Information Theory Group Seminar, University of Notre Dame, Notre Dame, Indiana, 1972.
34. *The Numerical Solution of the Boltzmann Equation in Three Dimensions*, by E. H. Bareiss, University of Illinois, Urbana, Illinois, 1972.
35. *The College Preparation for a Mathematician in Industry*, by E. H. Bareiss, Keynote address, Spring Meeting MAA, Southern Colorado State College, 1972.
36. *The Use of Interpolatory Polynomials for a Finite Element Solution to the Multigroup Diffusion Equation*, by A. J. Lindeman, American Nuclear Society, Las Vegas, Nevada, 1972.
37. *Static and Dynamic Numerical Characteristics of Floating Point Arithmetic*, by W. J. Cody, IEEE - TCCA Symposium on Computer Arithmetic, College Park, Maryland, 1972.
38. *A Combinatoric Division Algorithm for Fixed Integer Division*, by D. H. Jacobsohn, IEEE - TCCA Symposium on Computer Arithmetic, College Park, Maryland, 1972.
39. *A Single-Problem Comparison: PL/I*, by K. Dr̄itz, SHARE Conference, San Francisco, California, 1972.
40. *Computer Image Processing*, by J. W. Butler, Mississippi State University, State College, Mississippi.
41. *The Use of Interpolatory Polynomials for a Finite Element Solution of the Multigroup Diffusion Equation*, by A. J. Lindeman, University of Maryland, Baltimore, Maryland, 1972.

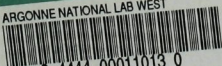
7.5 AMD Seminars

1. *A Numerical Comparison Between a Finite Difference Approximation and a Finite Element Approximation for the Two-Dimensional Multigroup Diffusion Equation*, by G. K. Leaf, Argonne National Laboratory, Argonne, Illinois.
2. *The Development of a Computerized Grade II Braille Translation Algorithm*, by L. C. Leffler and W. Lidinsky, Applied Mathematics Division, Argonne National Laboratory, Argonne, Illinois.
3. *Algebraic Mappings Related to the Lyapunov Quadratic Form Criterion for Stability*, by W. Givens, Applied Mathematics Division, Argonne National Laboratory, Argonne, Illinois.
4. *The IBM Proposal for a New Macro Language for PL/I*, by K. Dritz, Applied Mathematics Division, Argonne National Laboratory, Argonne, Illinois.
5. *Static and Dynamic Numerical Characteristics of Floating Point Arithmetic*, by W. J. Cody, Applied Mathematics Division, Argonne National Laboratory, Argonne, Illinois.
6. *The Thermal Structure of the Upper Two Millimeters of a Wavy Ocean*, by J. Witting, Office of Naval Research, Washington, D.C.
7. *Recent Developments in Efficiency in Machine Computation and Reduction of Linear Systems*, by D. Mazukelli, San Francisco State College, San Francisco, California.
8. *Defining Standard PL/I*, by M. D. MacLaren, Applied Mathematics Division, Argonne National Laboratory, Argonne, Illinois.
9. *A Run-Time System for PL/I on the CDC-6000*, by Milton Barber, Control Data Corporation, Palo Alto, California.
10. *Numerical Simulation of the Navier-Stokes Equations in Fourier Space*, by J. R. Travis, Reactor Analysis and Safety Division joint seminar, Argonne National Laboratory, Argonne, Illinois.
11. *Reduction of Group Representations*, by J. R. Gabriel, Applied Mathematics Division, Argonne National Laboratory, Argonne, Illinois.
12. *Multiple Shorting Procedures for Non-Linear Boundary Value Problems*, by R. Bulirsch, Mathematisches Institut der Universität zu Köln, Köln, Germany.
13. *On the General Concepts of Fields of Values (Numerical Ranges of Operators)*, by F. L. Bauer, Mathematisches Institut der Technischen Universität München, München, Germany.
14. *Crystallographic Computer Graphics and the ORTEP Program*, by C. Johnson, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

15. *Design for a Real-Time Critically-Ill Patient Monitoring System*, by S. S. Yau, Northwestern University, Evanston, Illinois.
16. *An Interactive Network Simulation System*, by C. W. Gear, University of Illinois, Urbana, Illinois.
17. *Fault Tolerant Computing*, by A. Avizienis, University of California, Los Angeles, California.
18. *EISPAC: Eigensystem Package Control Program*, by J. Boyle, Argonne National Laboratory, Argonne, Illinois.
19. *Image Processing: A Survey*, by C. B. Shelman, Argonne National Laboratory, Argonne, Illinois



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